The Role of Hydrogen Value Chains in Decarbonised Energy Systems
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The Role of Hydrogen Value Chains in Decarbonised Energy Systems

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DECLARATION OF AUTHORSHIP

This thesis is composed of my original work and contains no material previously published or written by another person except where due reference has been made in the text. The contributions by others to the journal articles used in this thesis are clearly stated in the thesis. The work published in the thesis was carried out since the commencement of my research degree at the University of Bath and does not include any other work submitted to qualify for another degree or diploma at any other institution.

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Abstract

Decarbonisation presents numerous challenges to energy systems. For example, renewable electricity sources such as wind and solar can provide low-carbon energy, but are variable, so new methods must be found to balance energy demand and supply. Furthermore, heating, transport and industry also require decarbonisation.

As a low-carbon and relatively energy-dense energy carrier, hydrogen could be used to aid energy decarbonisation, by providing electricity storage, as a transport fuel, heating buildings, or as a chemical feedstock. However, with multiple production pathways and applications, it is unclear how hydrogen should be implemented to provide the best support to decarbonisation. Modelling of energy systems can help to assess this.

In this thesis, a review of power-to-gas projects identifies the growing interest in hydrogen globally, and identifies key requirements for modelling hydrogen in energy systems. Hydrogen can provide energy flexibility in several different energy sectors, or even enable coupling between them. Therefore, hydrogen must be modelled with sufficient spatial, temporal and technological detail so that these synergies can be identified. This thesis argues that many influential global energy scenarios lack these details, which may explain the mixed coverage of hydrogen in the scenario results.

Value chain optimisation is used to explore how hydrogen can assist in energy decarbonisation. A value chain model of a national energy system is presented, and configured in the thesis in order to represent hydrogen and associated technologies within evolving energy systems. From data gathered from existing energy systems and emerging technologies, a series of scenarios are designed that explore the role of hydrogen in the supply, management and demand of energy.

The scenario results show that hydrogen could be valuable for providing flexibility to energy systems, for example balancing supplies and demands of electricity and moving energy between sectors and regions. However, bulk hydrogen production is relatively expensive, due to the costs of the energy feedstock, and losses in the conversion to hydrogen. Therefore the flexibility benefits of hydrogen may not be sufficient for it to be competitive in current markets. With policy support, for example in industry or for partial injection into gas grids, hydrogen supply chains could become established, and then hydrogen can begin to provide wider energy system benefits.

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Achievements

Article publications:

- Quarton, C. & Samsatli, S. Power-to-gas for injection into the gas grid: what can we learn from real-life projects, economic assessments and systems modelling? *Renewable & Sustainable Energy Reviews*, 98:302-316, 2018. DOI: 10.1016/j.rser.2018.09.007. IF 12.11.

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Other:

- Three six-week placements at the Department for Business, Energy & Industrial Strategy (BEIS), within the Science & Innovation for Climate and Energy Directorate (SICE). Placement dates: Jan-Feb 2018; Jan-Feb 2019; Jan-Feb 2020.

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Chapter 1

Introduction

Energy systems are undergoing significant changes in order to reduce greenhouse gas emissions and prevent catastrophic climate change. These changes will be challenging, and are likely to require a variety of new technologies and energy carriers. Hydrogen has significant potential for assisting with the energy transition, as it is a low-carbon energy carrier with attractive storage characteristics, and may be able to provide flexibility to energy systems.

It is unclear exactly how emerging low-carbon technologies should be implemented to achieve energy decarbonisation. Any energy transition should aim to achieve climate change ambitions, but at a low overall cost, and ideally with minimal other disruption, for example to consumers and the wider environment. The focus of this thesis is to use energy value chain modelling to understand how hydrogen may be used most effectively to assist in achieving these goals.

1.1 Context: new challenges and new technologies for energy systems

If catastrophic man-made climate change is to be prevented, the evidence suggests that a global average temperature rise of less than 1.5 °C should be targeted, and that countries will be required to achieve net greenhouse gas emissions of zero by at least the end of the century [1]. In the UK, the climate change act was amended in 2019, committing the country to achieving net-zero emissions by 2050 [2]. Primary energy usage accounts for over 70% of global greenhouse gas emissions [3, 4], so it is essential that energy systems are decarbonised if climate change targets are to be met.

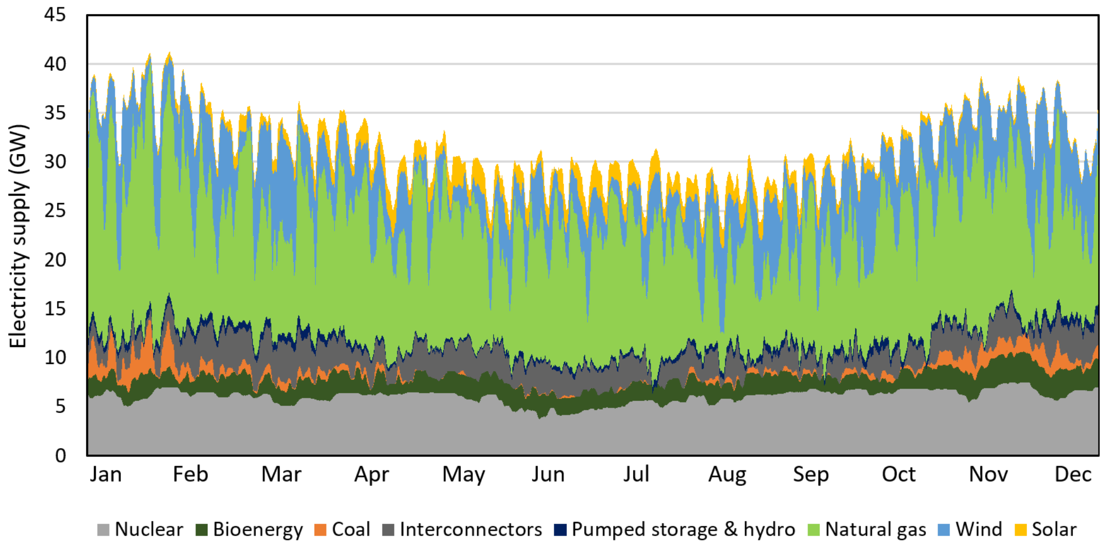

Figure 1-1: **Great Britain electricity generation by source in 2019.** Wind and solar make a significant contribution, but their intermittency is managed through a combination of dispatchable fossil fuels, pumped storage, and interconnectors. Data from [8].

Decarbonising energy systems is technically feasible, but will require a significant transition from the present day. Present-day systems still rely on fossil fuels, which are typically relatively low-cost, easy to manage, and dispatchable. But fossil fuels have associated greenhouse gas emissions, primarily from their combustion, but also throughout the supply chain [5].

Alternative energy technologies such as wind and solar electricity generation can be expected to contribute significantly to energy decarbonisation. These renewable energy sources cause no direct greenhouse gas emissions, although may have some supply chain emissions [5]. Costs for these technologies have fallen rapidly and are expected to fall further in future decades [6]. Already today these technologies make significant contributions to energy systems: Figure 1-1 shows the Great Britain (GB) electricity supply for 2019, where 20% of electricity was provided by wind and 4% by solar [7, 8].

However, there are a number of reasons why fossil fuels cannot be replaced by renewables like-for-like. Fossil fuels are relatively easy to store, and many can be dispatched when they are needed. For electricity generation for example, reserves can be stored and converted to electricity variably, in order to match variable electricity demands. Many renewable sources meanwhile, including wind and solar, are intermittent: electricity is only available when conditions are right (e.g. the wind is blowing or the sun is shining). In present-day systems, intermittent renewable generation is typically man-

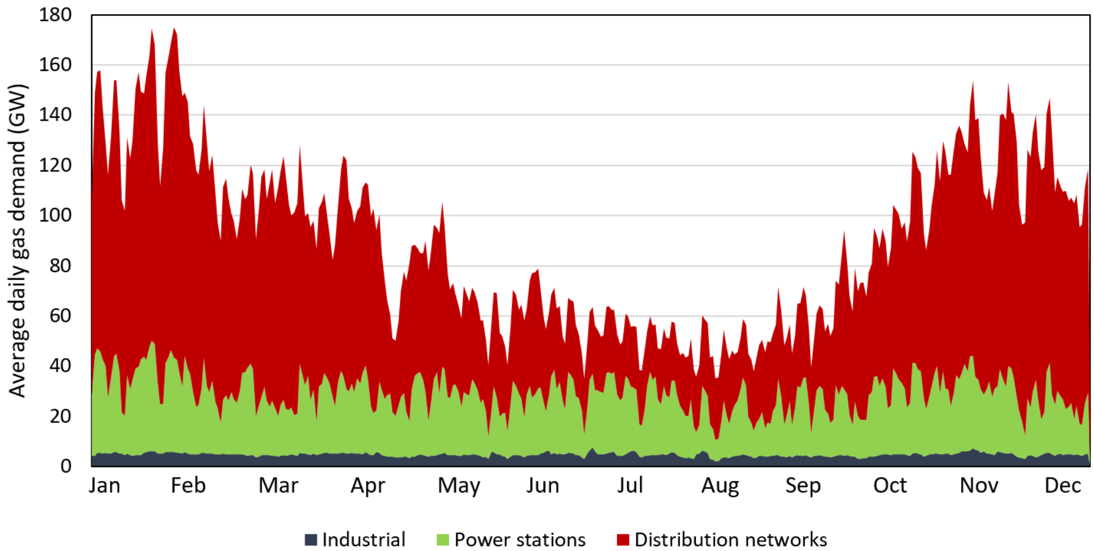

Figure 1-2: **Great Britain natural gas demands in 2019.** The data shown are the daily gas demands from the GB National Transmission System; shown as average demand in GW for comparison with Figure 1-1. Data from [11].

aged with flexible fossil fuel generation, ramping output in order to balance demand: Figure 1-1 shows that natural gas provides this service in the GB system.

Furthermore, energy decarbonisation is not restricted to electricity. Natural gas is a major energy carrier in many countries, supplying energy for power stations, industry, businesses and homes. In GB for instance, 86% of households are connected to the natural gas grid [9].

Figure 1-2 shows GB natural gas demands for 2019. Firstly, it can be seen that gas demands are significantly larger than electricity demands: annual gas demands in GB are typically around 880 TWh, compared to 300 TWh for electricity [10]. Secondly, gas demands, which are primarily driven by heating demands, are more variable than electricity demands. Various strategies are employed to manage this variability, including natural gas grids with inherent flexibility (linepack), and international natural gas supply chains. However, combustion of natural gas generates significant CO_2 emissions, so solutions need to be found to reduce demands for natural gas, or at least minimise the emissions generated by its use. Any solutions that are found will also need to be sufficiently flexible to satisfy the variable energy demands.

Ease of storage also makes fossil fuels valuable as transport fuels, in particular in applications such as aviation where energy density is critical. Finally, there are other applications where fossil fuels cannot simply be exchanged for electricity, for example

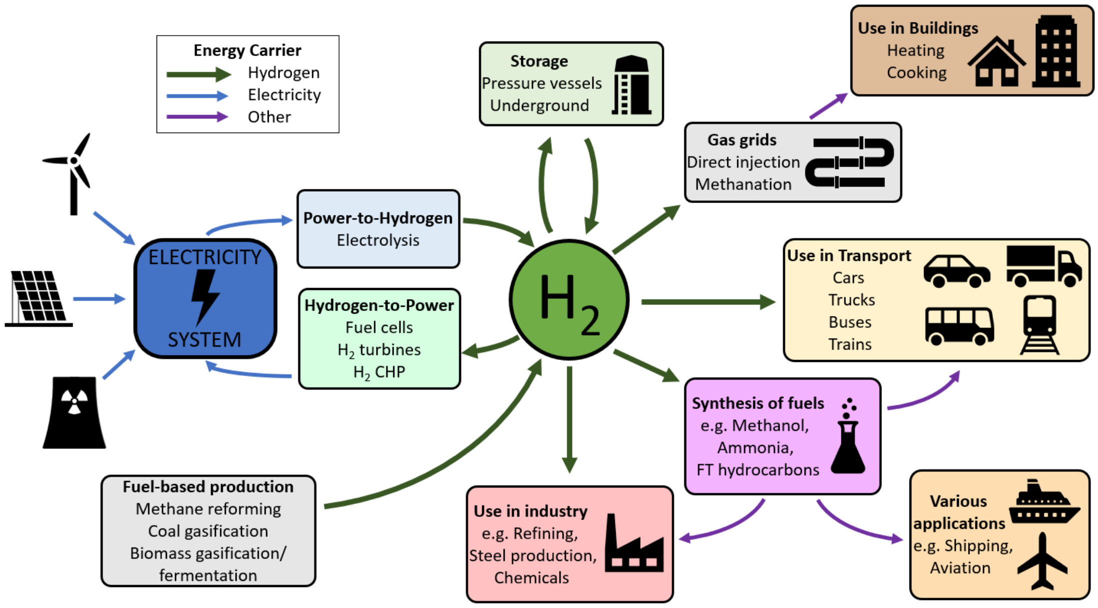

Figure 1-3: **Overview of key hydrogen production and usage pathways.** With multiple production options and applications, hydrogen could be valuable in providing flexibility and sector-coupling to energy systems. Figure replicated from Chapter 3.

in chemical feedstocks [12].

Hydrogen shows considerable potential for aiding energy decarbonisation and easing the transition away from fossil fuels. Figure 1-3 illustrates some of the options for how hydrogen could integrate with energy systems: more detailed introductions to hydrogen as an energy carrier are provided in Chapters 2 and 3. Whilst hydrogen is only naturally available in small quantities, it can be produced from other resources, including from electricity via electrolysis, and from biomass or fossil fuels [13]. Greenhouse gas emissions associated with these latter supply chains can be reduced through CO_2 capture and storage. There are no CO_2 emissions associated with the use of hydrogen as an energy carrier. Hydrogen itself has a global warming potential (estimated to be around 4.3 over 100 years [14]), and other greenhouse gases such as NOx may be produced through combustion of hydrogen; however emissions of these gases can be minimised with appropriate gas handling and equipment design [15].

Apart from the absence of CO_2 emissions, hydrogen shares many similarities with fossil fuels; methane in particular has many comparable characteristics. The energy content of fuels can be compared using the "heating value", which represents the heat released by combusting a specified quantity of the fuel. The "lower heating value" (LHV) assumes that all water that is produced remains as vapour, whilst the "higher heating value" (HHV) includes the heat recovered by condensing the water vapour that is produced. Hydrogen has a LHV of 120 MJ/kg, compared to 50 MJ/kg for methane.Hydrogen is also a gas at standard temperature and pressure, with an energy density of 10.8 MJ/m^3 (compared to 35.6 MJ/m^3 for methane). Therefore hydrogen may be able to fulfil some of the roles traditionally performed by fossil fuels in energy systems, such as large scale energy storage, use as a dispatchable fuel, and as an industrial feedstock. In this way, hydrogen may be able to complement renewable energy sources in decarbonised energy systems by providing system flexibility. Possible applications could include generation of hydrogen at times of excess energy supply, and consumption of hydrogen at times of excess demand. Hydrogen can also provide "sector-coupling" to energy systems: allowing for energy flows between different sectors, potentially unlocking new efficiencies [16].

There are challenges to using hydrogen in energy systems however. As hydrogen is not abundantly available as a natural resource, it must be produced from another energy resource such as electricity, fossil fuels or biomass. Therefore hydrogen supply chains are likely to require new energy technologies that have not previously been deployed at scale, and must be carefully designed to avoid high costs or CO_2 emissions.

Hydrogen is not the only option that could be used to aid energy decarbonisation, and it is likely that a mix of technology options will be used. A selection of other options that may have significant roles in future low-carbon energy systems includes CO_2 capture and storage; alternative energy storage technologies; demand-side response; and electrification of heating and transport [12].

Despite, or perhaps as a result of, the range of technology options available, the optimal pathway to a decarbonised energy system is unclear. An understanding of the "target" energy system could help to guide present-day decision making for policymakers and investors. For example, major obstacles or knowledge gaps could be identified, so that efforts can be made now to address them. Meanwhile, investment in technologies that in reality have little long-term potential could be avoided.

1.2 Energy value chain optimisation

In this thesis, the main approach that will be used to explore the energy system challenges described above is value chain optimisation. A value chain can be defined as "a network of technologies and infrastructures (such as conversion, transportation, storage) along with its associated activities (such as sourcing raw materials, processing, logistics, inventory management, waste management) required to convert low-value resources to high-value products and energy services, and deliver them to customers" [17]. Value chain or supply chain optimisation seeks to find an "optimal" design and operating strategy for this network, and was traditionally used in fields such as process systems engineering [18].

One of the early uses of supply chain optimisation for hydrogen is by Almansoori and Shah [19]. This model optimises the production and supply of hydrogen as a transport fuel, and has been the basis for multiple subsequent studies (e.g. [20, 21, 22]).

Samsatli and Samsatli developed the Value Web Model (VWM), in which value chain optimisation is applied not just to hydrogen for transport but also the wider energy system [23, 24]. This approach interprets energy systems as a series of interconnected value chains: or a "value web". These value chains cover the delivery of primary energy resources (such as wind or natural gas) to useful consumed energy (such as consumed electricity and heat in homes). A wide variety of technologies may be employed in these value chains for the conversion, storage, transportation and distribution of resources. Different energy resources, such as electricity or hydrogen, may be produced in different ways, and used at different stages of each value chain, resulting in an interconnected web.

Many other techniques have also been used to model energy systems. Well-known large-scale energy systems models, for example, include the MARKAL/TIMES modelling family [25, 26] and MESSAGE [27]. Various reviews of energy systems models have been performed (e.g. [28, 29, 30, 31]); more information on some of the alternative models is also provided in Chapters 2 and 3 of this thesis.

Value chain optimisation of energy systems can provide alternative perspectives and insights to these models. For example, value chain optimisation may be able to identify potential interactions between usually unconnected supply chains or sectors, thus identifying opportunities for "sector-coupling". Meanwhile, value chain optimisation may be able to model a level of detail not captured by large-scale economic models.

In this thesis, value chain optimisation will be used to explore the role of hydrogen within energy systems. The thesis will demonstrate the benefits of using the value chain approach, and the natural suitability of value chain optimisation for modelling "flexibility" technologies such as hydrogen.

1.3 Research objectives

The overall aim of the research is to understand how hydrogen may be used most effectively to assist in decarbonisation, in particular how it can be used to provide flexibility to energy systems. The primary method used will be energy value chain modelling. The overall research objectives can be described as follows:

1. Understand energy systems, the issues associated with decarbonisation, and the characteristics of hydrogen as an energy carrier;

2. Design and model scenarios exploring the role of hydrogen within energy systems;

3. Interpret model results to provide insights into the role of hydrogen within decarbonised energy systems.

The following subsections provide some more detail for each of these objectives.

1.3.1 Understanding energy systems and hydrogen

Understanding current and future energy systems and the characteristics of hydrogen will be essential for accurately modelling them. This will include understanding how various technologies and processes interact; practical and safety issues; costs; environmental impacts; and other societal issues. The characteristics of a system need to be well understood so that the modelling tool is designed appropriately, and a large set of input data needs to be acquired. In some areas, not all issues are yet fully understood: certain practical aspects of using hydrogen with existing natural gas infrastructures, for example. Developing an understanding of all issues will give the opportunity to summarise and review the latest findings and to inform the modelling work.

The scope of topics to be covered includes existing energy systems, and emerging technologies that may become important in the future, in particular hydrogen. Specific areas to study in detail include:

- The design and operation of key existing energy infrastructures. For example the existing GB gas grid, including its extent, costs and flexibility (linepack) capability;

- The various technologies for hydrogen production, including from electricity, biomass and fossil fuels. This includes resource requirements, costs, environmental impacts, operating parameters, and other practicalities;

- Management of hydrogen as an energy carrier, including the means of storing and transporting hydrogen;
- Other issues with hydrogen as an energy carrier, for example safety concerns with the use of hydrogen in the home;
- Practicalities of hydrogen injection into the gas grid, including both partial injection of hydrogen (blending) and complete conversion of existing gas grids to hydrogen;
- Other key technologies that are associated with hydrogen value chains, for example CO_2 capture and storage and renewable electricity generation;
- Wider societal issues with decarbonisation, such as public opinion, the policy landscape, and the economic outlook.

1.3.2 Design and model hydrogen scenarios

The second objective concerns the selection and configuration of a modelling tool, and the design of scenarios to be modelled. The modelling tool must be suitable for modelling the key characteristics of hydrogen; understanding what these requirements are will be achieved through a literature review. It is intended to use the Value Web Model for the modelling work, as it is a powerful tool that has already demonstrated its strengths in modelling hydrogen value chains within energy systems [23, 32, 33]. In this thesis, the Value Web Model will be configured to provide as detailed a representation of hydrogen technologies within the GB energy system as possible.

A series of scenarios will be designed to use with the Value Web Model. This will both demonstrate the functionality of the model, and provide insights regarding the role of hydrogen and other technologies throughout the energy transition. The scenario design is a key part of the modelling process: models require appropriate input data in order to generate valuable results. Scenario design will need to consider all of the topics described in Section 1.3.1, to ensure that accurate and relevant results are generated.

Due to the need to for high spatial, temporal and technological detail it will only be possible to model a limited number energy sectors and technologies in this thesis. The sectors and technologies that will be included will be those most relevant to the GB energy system, and most likely to develop valuable modelling insights.

Overall, the focus of this thesis is to consider the role of hydrogen in providing energy system flexibility. Therefore the applications that are of most interest are: hydrogen for electricity storage (for example absorbing excess renewable electricity), and hydrogen in the gas grid (where linepack flexibility can be exploited). As a result, the electricity sector is firmly within scope, including technologies associated with the generation, transportation and storage of electricity. Additionally, given that the primary function of the gas grid is to deliver gas for heating, the heating sector is also within scope, including technologies for converting electricity, natural gas and hydrogen to heat. As will be seen, initially only domestic demands for electricity and heat will be considered, but this scope will be expanded later in the thesis to include commercial and industrial demands.

The most prominent energy sector that is not modelled in this thesis is transport. This is primarily to retain a manageable scope for the modelling, but is also because the present-day transport sector, with mostly petroleum-focussed supply chains, is less integrated with the gas and electricity sectors. Whilst this is likely to change, with uptake of both electric and hydrogen powered vehicles creating opportunities for the transport sector to integrate with the rest of the energy system, this integration is beyond the scope of this thesis.

The exact list of energy technologies modelled in each scenario of this thesis may not remain constant, with different technologies being included depending on the scenario being explored, and increasing technological depth as the thesis progresses. Nevertheless each modelling chapter in this thesis includes details of which technologies were included for the scenarios in that chapter. Additionally, a full list of all technologies modelled in this thesis, including the data assumptions for each technology, is provided in Appendix B.

1.3.3 Interpreting model results to provide hydrogen insights

The final objective concerns interpreting model results in order to generate useful insights into the role of hydrogen. Key questions to answer will include:

- How will optimal decarbonised energy systems be designed?
  - Which technologies and value chains should be used?
  - What is the role of hydrogen in these systems: as a major energy carrier, providing a supporting (e.g. flexibility) role, or with no role at all?
  - Where will technologies be installed, and how will they operate?
  - Which energy feedstocks should be used and where will they come from?

- How should energy systems transition from the present day to fully decarbonised systems?
  - When should existing technologies and infrastructures be retired, and when should new technologies be installed?
  - What is the role of government policy in the system transition?
  - Is there a role for any transitionary technologies?
- How much will energy decarbonisation cost?
  - What are the relative costs of different decarbonisation options?
  - Who will bear these costs and how should they be managed?
  - What will be the cost of low-carbon hydrogen?

A large number of energy system modelling studies have been performed before and more will be performed in the future. The original contribution of this thesis arises from two aspects: the focus on hydrogen, whilst maintaining consideration and accurate representation of the wider energy system, and the methods used.

Few previous modelling studies have considered the detailed aspects of hydrogen as an energy carrier, whilst also accounting for the wider aspects of energy systems. Chapter 2, for example, reviews studies in which hydrogen as an energy carrier is modelled, but usually this is only through an economic business case study or an over-simplified energy model. Meanwhile in Chapter 3, some influential global scenarios are discussed that do consider the wider energy system, but the underlying models lack any detailed representation of hydrogen, so the resulting level of hydrogen in the scenario results is mixed. It is only through detailed representation of hydrogen, whilst also considering all aspects of the wider energy system, that all possible interactions can be considered and the value of hydrogen can accurately be assessed.

The application of a value chain optimisation approach to energy systems as a whole is a relatively new approach, and makes it possible to account for both the detail of hydrogen and the wider energy system. In this thesis, value chain optimisation will be used for specific applications where it has not been used before, including for detailed modelling of CO_2 value chains and modelling of gas transmission and distribution networks.

1.4 This thesis

This is an "alternative format" thesis, where journal articles are included in the main chapters of the thesis. In this thesis, the introduction and the conclusion are "conventional" chapters, but the five intervening chapters are based on journal articles. This format means that there is inevitably some repetition between chapters, for example with each chapter needing to set out the context of the research and basic principles of the modelling approach. However, each chapter builds on the preceding chapter to develop an overall body of research that achieves the objectives set out in Section 1.3. Narrative text, in the form of introductory and concluding remarks, is provided for each chapter. This text clearly outlines the contribution of the article to the overall thesis and highlights the connecting themes between each chapter.

Results and conclusions in each article in this thesis are based on the information available at the time the article was written, which due to the fast-moving nature of this field of research, may not always be fully up-to-date. The concluding remarks for each chapter attempt to provide up-to-date context for the chapter, but it is important that any future decisions (for example by policymakers) are made using the most up-to-date information available to them.

Each of the "article" chapters has the same structure:

- Chapter introductory remarks, providing some context for the article;
- Authorship declaration, stating the contributions of the co-authors of the article;
- Journal article, as published (or submitted), although re-formatted for this thesis;
- Reference list, as published (or submitted) with the original article;
- Chapter concluding remarks, expanding on the article findings in the context of this thesis.

Each article has its own reference list, and article citations are unchanged from the originally published (or submitted) articles. This introduction also has its own reference list at the end of the chapter.

Following this introduction, Chapter 2 contains an article published in Renewable and Sustainable Energy Reviews, detailing a literature review of power-to-gas, including real-life projects and modelling studies. The article provides a technical introduction to hydrogen as an energy carrier and the concept of power-to-gas, and a discussion of the the advantages and practicalities of injecting hydrogen into existing gas grids.

Initially, a brief review of all power-to-gas projects globally is provided, followed by a focussed review on power-to-gas for injection into the gas grid. The review of power-to-gas for the gas grid includes real-life projects and modelling studies. This allows a comparison of their scope, assumptions and outcomes, providing insights into the potential for hydrogen injection into the gas grid and the state-of-the-art for modelling this process. Overall, the study identifies the key requirements for modelling hydrogen injection into the gas grid, which will form a significant part of later chapters in this thesis. Finally, the chapter concluding remarks include an update to the review of power-to-gas projects, given that the original review article was published in 2018.

Chapter 3 presents a perspective paper published in Sustainable Energy and Fuels, in which the role of hydrogen in global energy scenarios is explored. A further introduction to the potential value of hydrogen in energy systems is provided. The article finds that the representation of hydrogen in global energy scenarios is mixed, and argues that this is partly due to deficiencies in the models and scenario designs used. The paper also makes suggestions regarding how such scenarios should be developed in order to represent hydrogen technologies more accurately and reliably. In addition to a thorough introduction to hydrogen as an energy carrier, this chapter provides valuable insights into the challenges of modelling energy systems that are under transition from centralised, fossil fuel based systems to diverse, flexible, low-carbon systems. These insights continue to highlight the modelling methods that will be essential for reliable modelling of hydrogen in later chapters.

The articles in Chapters 4 to 6 present the modelling work that was completed for this thesis. The chapters are presented in the order that the work was carried out. Each chapter represents a development in the depth and breadth of the scenarios modelled in the Value Web Model. By modelling and presenting energy scenarios, questions regarding the potential and challenges for hydrogen within energy systems can be explored, whilst also demonstrating the functionality of the model.

Chapter 4 presents an article that was published in Applied Energy. This article includes an introduction to the Value Web Model including the model scope, key constraints, and objective function. As part of this study, the Value Web Model was extended, including the representation of CO_2 as a resource that can be utilised in different processes (rather than merely as a waste flow). This allows for the modelling of CO_2 capture, utilisation and storage (CCUS) technologies, which are key aspects of several hydrogen value chains. The scenarios modelled in the article also provide interesting insights into the role for CCUS and hydrogen in decarbonising domestic heat and electricity.

Chapter 5 presents an article that has been published in Applied Energy. In the article, a detailed discussion of the advantages and practicalities of injecting hydrogen into gas grids is provided, including calculations of the effects of hydrogen injection on pipeline energy delivery rate and linepack flexibility. Following this, a much more detailed representation of gas networks is modelled in the Value Web Model, including representation of hydrogen injection into the gas grid. Scenarios with hydrogen injection in the GB energy system are modelled, including assessing the impacts of feed-in tariffs on the uptake of hydrogen injection.

In Chapter 6, an article is presented that is currently under review with Sustainable Production and Consumption. The article builds on the modelling methodology that has been developed in the previous chapters, and models a set of scenarios that explore the role of hydrogen under a range of policy interventions. This allows for a deeper study of the optimal use of hydrogen value chains within the energy system, and also considers the costs to consumers of different decarbonisation pathways.

Finally, the conclusion provides: a brief summary of the research findings from the previous chapters; a discussion of the role of hydrogen in decarbonised energy systems; and recommendations for further research and for innovation and policy.

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Chapter 2

Literature review: Power-to-gas and gas grid injection

Chapter introductory remarks

This chapter is based on the review article published by Elsevier in Renewable and Sustainable Energy Reviews. The article was published as open access, permitting reproduction in any medium, provided the original work is cited. The original article reference is as follows:

> Christopher J. Quarton and Sheila Samsatli. Power-to-gas for injection into the gas grid: what can we learn from real-life projects, economic assessments and systems modelling? *Renewable and Sustainable Energy Reviews*, 98:302-316, 2018. https://doi.org/10.1016/j.rser.2018.09.007

The article is a literature review, carried out in 2017-18 as the main literature review for this thesis. The review assesses the status of power-to-gas, with a particular focus on power-to-gas for injection into the gas grid. The review considers both modelling of power-to-gas and gas grid injection, and real-life power-to-gas projects.

Reviewing power-to-gas modelling studies was important to understand the existing state of modelling in this area. As the results of the review show, several studies have modelled power-to-gas and gas grid injection in some form, but a wide variety of modelling approaches have been used, with differing assumptions. Therefore by collating these methods and assumptions, this review was able to highlight any discrepancies, and identify the key requirements for the modelling work in this thesis.

Reviewing real-life projects was considered to be valuable for a number of reasons. The field of power-to-gas has had considerable interest in recent years, with rapid growth in the number of projects in planning and operation. Whilst reviews of power-to-gas projects had been performed before, this review provided a chance to update these with the latest projects. A focus on projects with gas grid injection was also valuable as it enabled the comparison of the assumptions made in modelling studies with real-life experience.

Following this introduction, an authorship declaration is provided, followed by the article as published in Renewable and Sustainable Energy Reviews (although re-formatted for this thesis). The article includes its own reference list.

Finally, some concluding remarks are provided. Included with those remarks is an update on the review of real-life projects. As has been mentioned, there is considerable growth in the field of power-to-gas, and the review article was published in 2018. Therefore it is valuable to assess the progress of the projects included in the review article, as well as to consider any new projects that have been announced since the article was published. The references that were used in this commentary text are listed at the end of the chapter.

Authorship declaration

<table>
<tr><td colspan="4">This declaration concerns the article entitled:
Power-to-gas for injection into the gas grid: What can we learn from real-life projects, economic assessments and systems modelling?</td></tr>
<tr><td colspan="4">Publication status
Draft manuscript ☐ Submitted ☐ In review ☐ Accepted ☐ Published ⊠</td></tr>
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<tr><td>Candidate's contribution to the paper</td><td colspan="3">The candidate contributed to / considerably contributed to / predominantly executed the...
Formulation of ideas:
60% - S. Samsatli and Dr Ian Llewellyn (BEIS supervisor) established the basic research question for the project. S. Samsatli and I jointly developed the specific focus for this literature review.
Design of methodology:
70% - I decided the review methodology and structure, with assistance from S. Samsatli.
Experimental work:
95% - I carried out the literature review, including the literature search and reading. S. Samsatli suggested a few references and provided insights.
Presentation of data in journal format:
80% - I structured and wrote the article, and designed all of the figures. S. Samsatli provided comments on the draft, made final edits to the manuscript for submission to the journal and helped address the reviewers' comments.</td></tr>
<tr><td>Statement from candidate</td><td colspan="3">This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.</td></tr>
<tr><td>Signed</td><td></td><td>Date</td><td>16/11/2020</td></tr>
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Article:

Power-to-gas for injection into the gas grid: What can we learn from real-life projects, economic assessments and systems modelling?

Abstract

Power-to-gas is a key area of interest for decarbonisation and increasing flexibility in energy systems, as it has the potential both to both absorb renewable electricity at times of excess supply and to provide backup energy at times of excess demand. By integrating power-to-gas with the natural gas grid, it is possible to exploit the inherent linepack flexibility of the grid, and shift some electricity variability onto the gas grid. Furthermore, provided the gas injected into the gas grid is low-carbon, such as hydrogen from renewable power-to-gas, then overall greenhouse gas emissions from the gas grid can be reduced.

This work presents the first review of power-to-gas to consider real-life projects, economic assessments and systems modelling studies, and to compare them based on scope, assumptions and outcomes. The review focuses on power-to-gas for injection into the gas grid, as this application has specific economic, technical and modelling opportunities and challenges.

The review identified significant interest in, and potential for, power-to-gas in combination with the gas grid, however there are still challenges to overcome to find profitable business cases and manage local and system-wide technical issues. Whilst significant modelling of power-to-gas has occurred, more is needed to fully understand the impacts of power-to-gas and gas grid injection on the operational behaviour of the gas grid, taking into account dynamic and spatial effects.

Abbreviations: $\%_{\text{HHV}}$: Efficiency based on higher heating value; CAPEX: Capital expenditure; CCS: Carbon capture and storage; CHP: Combined heat and power; CO_2: Carbon dioxide; HIGG: Hydrogen injection into the gas grid; LP: Linear programming; MIGG: Methane injection into the gas grid; MILP: Mixed-integer linear programming; MINLP: Mixed-integer nonlinear programming; NFCRC, National Fuel Cell Research Centre; NLP: Nonlinear programming; OPF: Optimal power flow; P2G: Power-to-gas; PEM: Proton exchange membrane; SMR: Steam methane reforming; Vol.%: Percentage blend by volume.

2.1 Introduction

Power-to-gas (P2G) is a key area of interest for decarbonisation and increasing flexibility in future energy systems, due to its potential to help integrate high penetrations of renewable energy. Combining P2G with the gas grid, primarily through direct injection of hydrogen, is one of several possible applications of P2G, and it has its own advantages and challenges.

When hydrogen is combusted it releases no carbon dioxide (CO_2) emissions; consequently any addition of hydrogen to the natural gas grid will result in lower CO_2 emissions at end use [1]. Provided the hydrogen is produced in a low carbon manner – either through steam methane reforming (SMR) with carbon capture and storage (CCS) or through electrolysis of "green" electricity – then overall CO_2 emissions will also be reduced. Many countries, such as the UK and the Netherlands, have extensive gas grids and there is interest in finding ways to continue to make of use these networks in a low carbon future, to avoid having to abandon these valuable assets altogether [2]. Furthermore, due to the ability of the gas grid to handle a range of gas pressures, it has an in-built flexibility which could be exploited by P2G, shifting some variability caused by intermittent renewables on the electricity grid onto the gas grid [3].

Nonetheless hydrogen injection into the gas grid (HIGG) has technical, economical and systems-level challenges [2, 4, 5]. Considerable work has been undertaken to understand these challenges through research, modelling and real-life demonstrator projects, and some effort has been made to establish a coordinated approach to expanding HIGG, for example through the HYREADY project [6]. However, many academic, industrial and policy studies have called for more to be done, particularly from policy-makers [2, 7, 8, 9, 10, 11].

Several reviews of P2G have been performed before. Schiebahn et al. [12] performed a technological review of power-to-gas with respect to the gas grid, including the technologies involved in the production, distribution and end use of the gas. Some reviews, including Haeseldonckx and D'Haeseleer [13], Dodds and Demoulin [14] and Götz et al. [15], have taken a broader assessment of P2G and the gas grid, assessing both the technological and wider system challenges. However, of these only Haeseldonckx and D'Haeseleer [13] considered partial HIGG: Dodds and Demoulin [14] considered a complete conversion of the gas grid to hydrogen, and Götz et al. [15] only considered synthetic methane injection into the gas grid (MIGG). Many similar studies have also been performed by private firms and regulatory and policy-making bodies [1, 2, 4, 16, 17]. The NaturalHy project [5] was a major study commissioned by the

European Commission which assessed the practicalities of delivering hydrogen in the European natural gas network, considering production, transport and end use.

Reviews of real-life P2G projects have also been performed. Gahleitner [18] performed a wide-ranging study of P2G projects and found that there was a focus of projects in Germany, but that projects had not been running long enough to draw specific conclusions on performance. Garcia et al. [19] conducted an expert opinion analysis of the potential of renewable hydrogen storage systems in Europe, including highlighting significant projects. Bailera et al. [20] reviewed 46 projects, but only considered power-to-methane.

Various approaches have been used to model P2G, but very few reviews of P2G modelling methods and their results have been performed. Typically, reviews that have been performed focus on general energy systems modelling techniques, with no interest in P2G. For example, Connolly et al. [21] reviewed models with a focus on integrating renewables into energy systems; Hall and Buckley [22] reviewed models in the UK context; and Pfenninger et al. [23] reviewed energy system models, questioning what the requirements are for these models in the twenty-first century. Blanco and Faaij [24] and Robinius et al. [25] both reviewed studies which included P2G, but only as one of a number of flexibility options, and were only concerned with the study results, not the modelling techniques.

The aim of this work is to provide a review of P2G and HIGG that for the first time considers both real-life projects and modelling studies and compares them based on scope, assumptions and outcomes. Furthermore, the interaction of P2G with the gas grid, primarily through HIGG, is of specific interest, due to the unique technical, economic and modelling characteristics associated with it. Inevitably, many P2G projects and studies include multiple P2G applications, so these are given consideration where necessary. MIGG is an alternative, or possibly complementary, pathway to HIGG which has its own set of strengths and weaknesses that are also assessed where appropriate.

The methodology comprises three elements:

1. An examination of over 130 reported real-life P2G and HIGG projects worldwide, in order to understand the historical trend in the scale and types of technology employed, as well as the types of application and the global distribution of the projects to identify what the impacts of P2G and HIGG are and where they are taking place;

2. An investigation of economic assessment studies performed for P2G and HIGG, comparing the different assumptions made about the level of hydrogen injection

allowed, identifying specific business cases for the technologies and assessing the resulting levelised cost and the wider system cost; and

3. An evaluation of energy systems models that considered P2G and/or HIGG and classifying them based on: the modelling approach employed; how the gas-electricity interface, storage and linepack were represented; how the spatial and temporal dependencies of system properties were captured; and what the objectives and the key design decisions of the models were.

The results from the three steps above were synthesised and categorised based on the scope, assumptions and outcomes of this wide range of studies, in order to obtain insights about the current status of the technologies and make recommendations for future research.

The remainder of this paper is structured as follows. Section 2.2 discusses the practical issues concerning producing hydrogen, injecting into the transmission and distribution gas grids, and its end use. Section 2.3 surveys the P2G projects worldwide, with a focus on HIGG projects. Following that is a literature review of modelling studies on P2G with a focus on HIGG: Section 2.4 reviews economic studies with an interest in the costs and business potential of HIGG, and Section 2.5 surveys studies that have used optimisation to assess P2G and HIGG from a whole system perspective. Finally, Section 3.4 summarises and compares the scope, assumptions and outcomes of the real-life projects and modelling studies.

2.2 Practicalities of P2G and HIGG

The following section provides a brief summary of the pathways and technologies of power-to-gas. A large number of studies and reviews have been carried out in this area: Schiebahn et al. [12] and Haeseldonckx and D'Haeseleer [13] are particularly recommended for more detail on this subject.

2.2.1 Production

Figure 2-1 shows an overview of the gas grid injection pathways, including power-to-gas. Hydrogen can be produced from electrolysis or SMR, and injected directly into the gas grid. Provided that the electricity source used for electrolysis is low-carbon, such as wind or solar energy, electrolysis has very low environmental impact. There are many references available for details of the electrolysis process [12, 26, 27]. Several

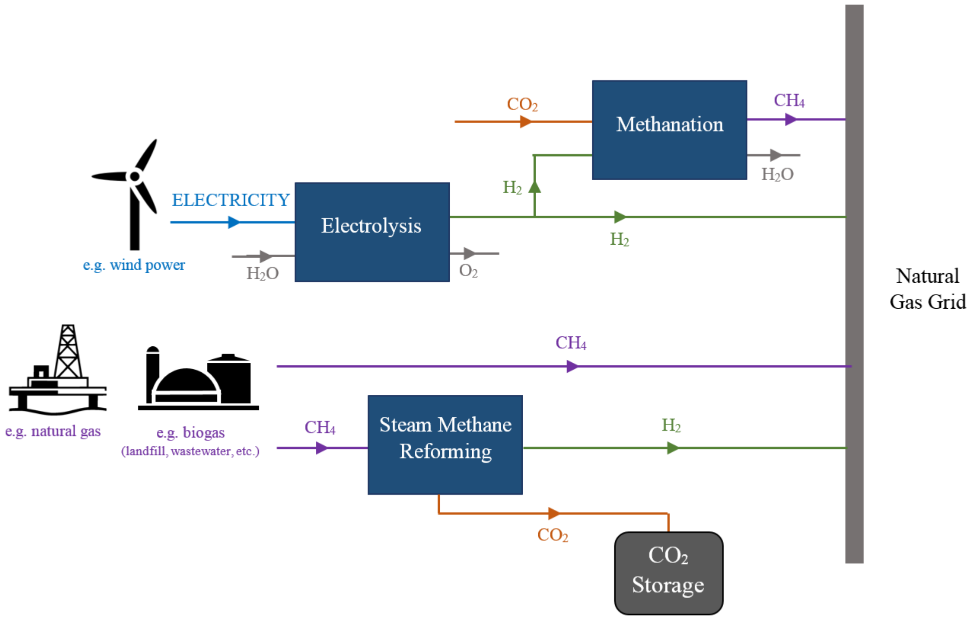


Figure 2-1: **Gas grid injection pathways, including: power-to-gas; hydrogen from steam methane reforming; direct injection of natural gas and biomethane; and synthetic methane from methanation of hydrogen.**

different electrolysis technologies exist and are used in P2G applications, as each has its own advantages and disadvantages. The most common technologies are: alkaline; proton exchange membrane (PEM); and solid oxide. Alkaline and PEM electrolysis have been used commercially for several decades in industrial applications. In recent years, manufacturers have also begun to produce commercial alkaline and PEM electrolysers capable of the more flexible operation regimes associated with P2G, although so far at a smaller scale [28]. Although solid oxide technology has been in development since the 1970s, it is less commercially established, mostly at the demonstration or pre-commercial stage [28, 29]. The technologies and sizes of P2G projects are discussed further in Section 2.3.1.

Alternatively to direct injection, hydrogen can be combined with CO_2 to produce methane, by methanation (for example using Sabatier synthesis [30]). Methane is a versatile and easy to store substance, and it forms the majority of natural gas [31], however when used as an energy source the CO_2 will be re-released. There is considerable interest in power-to-methane as it has fewer barriers to implementation than power-to-hydrogen. However, its potential for significantly reducing CO_2 emissions in the long term is limited.

2.2.2 Distribution and transmission

A concern with direct injection of hydrogen into the natural gas network is hydrogen embrittlement, which can occur in pipes made of iron and steel, and can lead to propagation of cracks in the pipework [32]. It is broadly agreed that hydrogen can be injected into the distribution network at a low concentration with no serious safety issues. Although the exact level is disputed, several studies suggest that up to 15–20% hydrogen blend by volume (vol.%) should be allowable [4, 5, 13]. Meanwhile, many regulators have seemingly arbitrarily low allowances on the amount of hydrogen in the blend. In the UK for instance the allowable limit is 0.1 vol.%, whilst in the Netherlands up to 12 vol.% is permitted [17]. Nowadays, polyethylene, which is not susceptible to hydrogen embrittlement, is being used more commonly in distribution networks. In the UK, for example, a major scheme is underway to replace iron gas pipes in the distribution grid with polyethylene (the Iron Mains Replacement Program), for safety reasons unrelated to hydrogen [33].

High pressures are thought to worsen the effects of hydrogen embrittlement, so it is generally agreed that allowable levels in high pressure transmission grids, which are often made from high strength steel, would be considerably lower than for distribution grids. Should transmission of hydrogen by pipeline over longer distances be required, it is possible that a purpose built pipeline network would need to be built [14]. Another concern which has been raised regarding transporting hydrogen in existing gas grids is the propensity of hydrogen to leak. However, several studies have concluded that leakage rates would not be high enough to be a major concern [5, 16].

Adding hydrogen to natural gas pipelines reduces the energy delivery of the pipeline. The effects are nonlinear and depend primarily on the energy density by volume and the flow properties of the hydrogen. As hydrogen is also less compressible than natural gas, the effect becomes more pronounced at higher pressures [1]. Figure 2-2 shows the energy delivery of pipelines at low and intermediate pressure levels with increasing levels of hydrogen injection, compared to if the pipeline delivered pure methane. In order to manage the reduced energy delivery in gas networks, either peak energy demand would need to be reduced, or higher flowrates (causing larger pressure drops) would be required [3].

2.2.3 End use

Gas from the distribution grid is most commonly used in homes for cooking or heating. In the UK for example, 86% of homes are connected to the natural gas grid [2]. Further

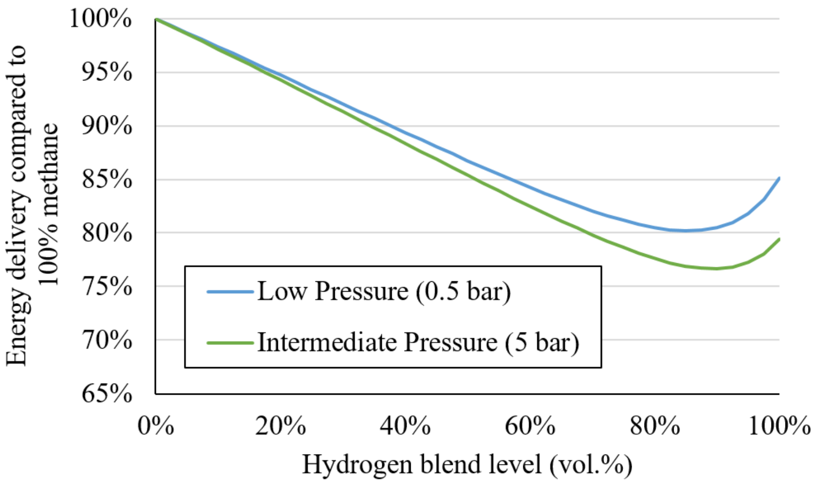


Figure 2-2: **Effect of hydrogen blend level on the energy delivery of gas pipelines** (based on the relationships presented in Abeysekera et al. [34])

safety concerns arise when considering hydrogen in the home, particularly regarding leakage and risk of ignition. For example, hydrogen has a higher risk of ignition than natural gas, and as with natural gas, it may be necessary to add an odorant to hydrogen to improve detectability. It may also be necessary to add a colourant, as unlike natural gas, a pure hydrogen flame is almost invisible [4]. Multiple studies have considered the effect hydrogen would have on the performance of household appliances, notably the NaturalHy project [5, 35]. Whilst most modern appliances should be capable of burning hydrogen blends of up to 20 vol.% [4], above this level it is likely that appliances would need adjusting or replacing, which would be a major undertaking [14, 36].

Besides in the home, the other major uses of natural gas are in power generation and industry. These facilities are more likely to be connected to high pressure pipelines or have their own direct supply of natural gas. Introducing hydrogen blends into combustors for equipment such as gas turbines will alter the combustion characteristics. However, a considerable amount of work has been performed in recent years to design burners suited to these characteristics. Although a gas supply with a time-varying hydrogen blend level would present additional challenges, work is ongoing to overcome these challenges [37].

2.3 P2G and HIGG projects worldwide

2.3.1 Overview of P2G projects

A review of P2G projects worldwide was performed based on several references. In addition to Gahleitner et al. [18], Garcia et al. [19] and Bailera et al. [20], screenings performed by both Iskov and Rasmussen [38] and Vartiainen [39] were used. Additionally the European Power-to-Gas Platform [40], containing a database of past, current and planned P2G projects in Europe was used. Only projects which include on-site electrolysis were considered, and projects producing hydrogen solely for transport, such as refuelling stations, were excluded. According to the website H2stations.org [41], at the beginning of 2018 there were 328 hydrogen refuelling stations worldwide but many of these do not produce hydrogen through on-site electrolysis. Nonetheless plants that produce hydrogen for transport in addition to other applications were included in the review. Electrolysis has been used to produce hydrogen for industrial applications since 1940 [42] – these historic projects were not included due to a lack of literature. Based on these references and criteria, over 130 P2G projects were identified worldwide.

Figure 2-3 shows the number of P2G projects that began operation in each year since 1990. After a small number of projects in the 1990s, increasing interest in P2G can be seen throughout the 2000s and 2010s. A breakdown of new electrolyser technology type per year is also shown. As can be seen, alkaline and PEM technologies dominate, with alkaline electrolysis being used in the majority of early projects, and PEM technologies growing in popularity more recently. Today, the two technologies have comparable performance characteristics and specific project requirements tend to determine the technology choice. Six projects have employed solid oxide technology, all intending to demonstrate the functionality of the technology and the wider system. These projects either use the reversibility of the solid oxide technology (operating in both electrolysis and fuel-cell mode) [43]; co-electrolysis (to produce synthetic natural gas or liquid fuels) [44, 45, 46]; or both of these functionalities [47, 48]. Regarding future projects (from 2018 onwards), it is likely that additional projects are in planning for which no literature was found.

The average size (electrolysis capacity) of new projects each year is also shown in Figure 2-3, with a clear upward trend. Figure 2-4 also illustrates project sizes by categorising them by size and operational status. Electrolysis capacity is used as the measure of plant size rather than hydrogen output, as the data are more easily available. According to a market survey by Buttler and Spliethoff [28], individual alkaline electrolyser stacks are available up to a capacity of 6 MW, whilst PEM stacks are typically smaller,

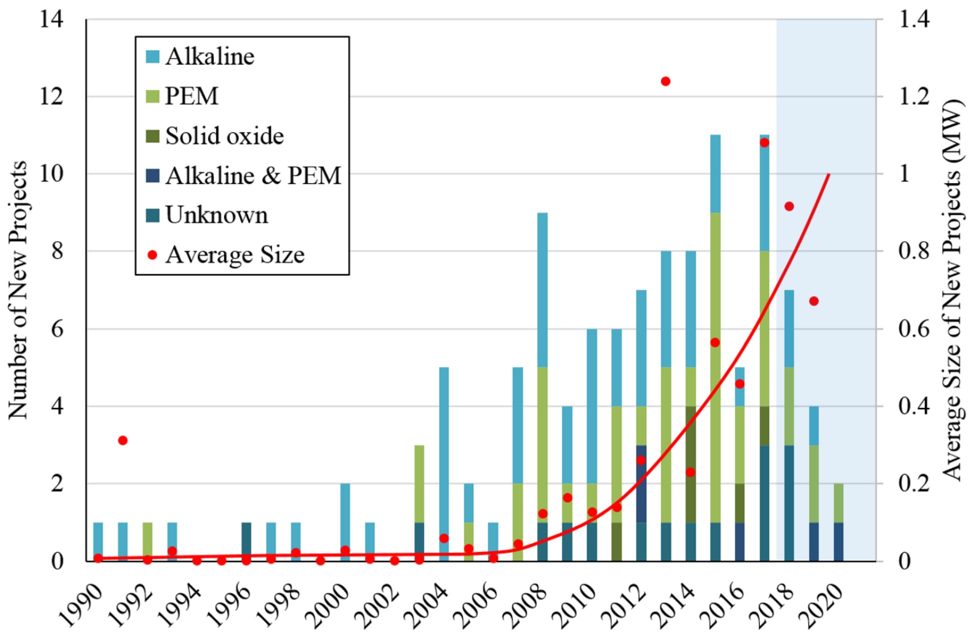


Figure 2-3: **Timeline of power-to-gas projects going into operation** (data obtained from [18, 19, 20, 38, 39, 40]). Data for 2018 onwards (shaded) is for known planned projects only; the actual number of new projects is likely to be higher.

with capacities of up to 2 MW. However, it is possible to install multiple electrolyser stacks at a single site, achieving overall electrolysis capacities of multiple megawatts using either technology. In addition to offering "nominal" capacities which can be maintained for continuous operation, electrolyser manufacturers commonly offer higher "peak" capacities for short term operation, a useful feature for grid balancing [17].

Almost half (43%) of all projects reviewed had an electrolysis capacity of less than 100 kW, however all planned projects are at least 0.5 MW in size. The largest plant in operation is the Audi e-gas plant in Werlte, Germany [18, 20, 49]. The plant has three electrolysers with a total capacity of 6.3 MW. The electrolysers are operated variably, powered by wind, and the hydrogen is used to produce methane which is injected into the gas grid (MIGG). The planned H2V Product project in France is far bigger, with 100 MW of electrolysis planned for HIGG [50, 51]. This project is discussed in more detail in Section 2.3.2.

Figure 2-5 shows the countries in which all completed, operational and planned projects are located. Germany leads in all of these categories, hosting over a third of all of the P2G projects that were identified. The USA has hosted a significant number of finished or currently operational projects, but all of these are of quite a small size, and no planned projects in the USA were identified at all. Many countries, predominantly

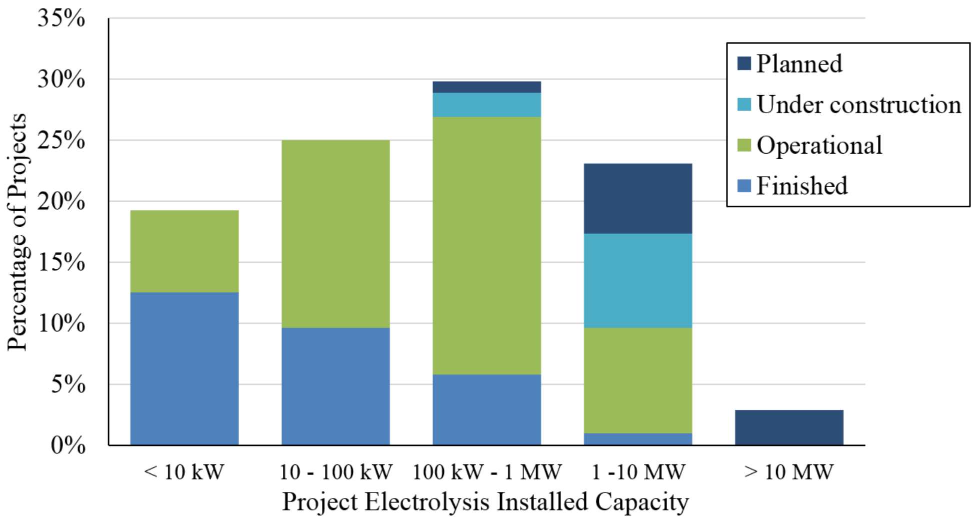


Figure 2-4: **Nominal electrolyser capacities of the projects examined in this paper** (data obtained from [18, 19, 20, 38, 39, 40]).

located in Europe and including the UK, have between four and nine projects either completed, operational or planned. Fifteen other countries (including Greenland) were identified which host three projects or fewer, meaning that twenty-six countries were covered in total.

Figure 2-6 shows the functions of all of the P2G projects identified. As can be seen, many projects have multiple functions (such as power and heat). Despite the low round-trip efficiency, over half of all projects include power-to-power functionality. The majority of these projects use hydrogen as a storage medium to provide a more stable power supply from renewable energy – either in a micro-grid setup where a small community relies on a local renewable electricity supply, or for wind farms connected to the grid aiming to provide a more stable electricity output. Despite transport-only plants being excluded from the review, still 18% of projects include delivery of hydrogen as a transport fuel as an additional functionality. Injection into the gas grid is another common function of the projects: 19% inject hydrogen directly whereas 8% inject methane. Other common uses for the hydrogen are for heating and as an industrial feedstock.

2.3.2 HIGG projects

Twenty-five projects were found that include HIGG, which represent 18% of the P2G projects that were reviewed. The details of these projects are summarised in Table 2.1.

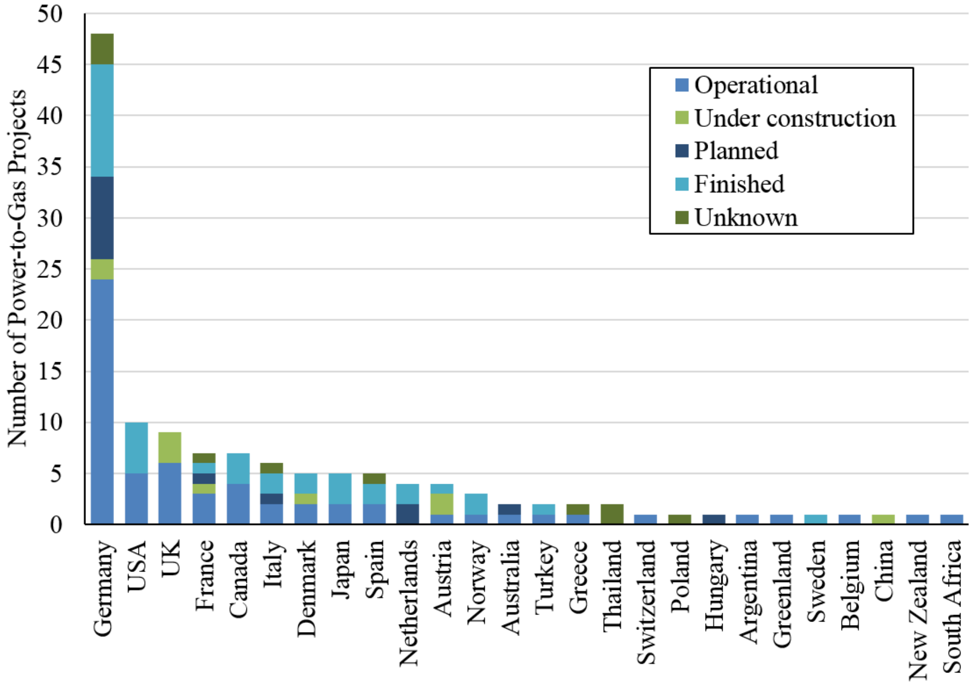


Figure 2-5: **Locations of power-to-gas projects** (data obtained from [18, 19, 20, 38, 39, 40]).

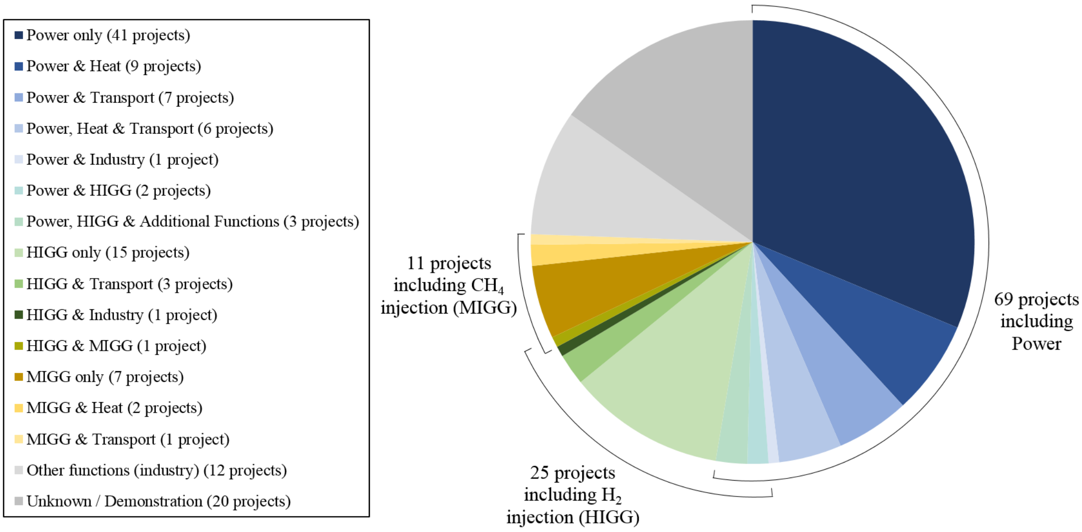


Figure 2-6: **Breakdown of the functions of power-to-gas projects** (data obtained from [18, 19, 20, 38, 39, 40]). Note that due to the very large numbers of transport-only projects that have been carried out, they were not included in the diagram. "Demonstration" refers to projects whose sole purpose was the demonstration of the technology, with no specified outlet for the hydrogen.

Table 2.1: Power-to-gas projects that include hydrogen injection to the gas grid

Project	Start Date	Status	Electrolyser Type	Size (kW, nominal)	References
Lolland Hydrogen Community, Denmark	2007	Operational	PEM	104	[18, 38, 39, 40, 52]
P2G Ameland, Netherlands	2008	Finished	PEM	8.3	[38, 39, 40, 53]
P2G Frankfurt - Thuga, Germany	2013	Finished	PEM	315	[39, 40, 54]
WindGas Falkenhagen, Germany	2013	Operational	Alkaline	2000	[18, 38, 39, 40, 55]
P2G NFCRC, USA	2014	Finished	PEM	67	[56, 57]
Hybrid Power Plant Enertrag, Germany	2014	Operational	Alkaline	500	[18, 19, 38, 39, 40, 58]
Energiepark Mainz, Germany	2015	Operational	PEM	3750	[39, 40, 59]
WindGas Hamburg, Germany	2015	Operational	PEM	1000	[19, 38, 39, 40, 60]
Hybridwerk Solothurn, Switzerland	2015	Operational	PEM	350	[20, 40, 61]
RWE Ibbenbüren, Germany	2015	Operational	PEM	150	[38, 39, 40, 62]
Wind2Hydrogen, Austria	2015	Operational	PEM	100	[19, 40, 63]
H2BER, Germany	2015	Operational	Alkaline	500	[39, 40, 64]
P2G Hassfurt, Germany	2016	Operational	PEM	1250	[39, 40, 65]
GRHYD, France	2017	Operational	Alkaline	Unknown	[19, 38, 39, 40, 66, 67]
Wind to Gas Südermarsch, Germany	2018	Operational	PEM	2400	[40, 68]
Kidman Park, Australia	2018	Planned	Unknown	Unknown	[69]
Jupiter 1000, France	2018	Under construction	Alkaline & PEM	1000	[39, 40, 67, 70]
HPEM2GAS, Germany	2019	Planned	PEM	180	[71]
HyDeploy, UK	2019	Under construction	PEM	500	[40, 72]
H2V Product, France	2021	Planned	Alkaline	100000	[50, 51]
P2G Ontario, Canada	Unknown	Under construction	PEM	2000	[73]
P2G Hanau, Germany	Unknown	Operational	PEM	30	[40, 74]
RH2-PTG, Germany	Unknown	Planned	Unknown	Unknown	[39, 75]
Storag Etzel, Germany	Unknown	Planned	Unknown	6000	[40, 76]
P2G Wyhlen, Germany	Unknown	Planned	Alkaline	1000	[40, 76]

There have been a few projects investigating the effects of HIGG on the pipelines and end use appliances. The first was the Lolland Hydrogen Community project [52], although rather than using an existing gas grid, a purpose-built pipeline network was constructed to supply pure hydrogen to 40 homes. Each home was fitted with a micro-combined heat and power (CHP) unit which used the supplied hydrogen for heating and electricity. Up to 20 Nm^3/h of hydrogen could be supplied by the PEM electrolyser. A project with a similar scope began in 2008 in Ameland in the Netherlands [53]. Fourteen homes in an apartment block were supplied with gas for heating and cooking. A PEM electrolyser was installed which could produce up to 1.05 Nm^3/h of hydrogen, and at its maximum, up to 20 vol.% hydrogen was injected. No effects from the hydrogen were detected in any of the pipework, the standard boilers and cookers that were used in the homes passed all of the safety tests and no issues were identified during operation. The National Fuel Cell Research Centre (NFCRC) in California, USA, are carrying out a small HIGG research project [56, 57]. A 7 kW PEM electrolyser is connected to a solar PV supply, in order to assess the operational performance of the system under variable electricity supply. A 60 kW electrolyser was also installed which supplies hydrogen to be injected into a small "off-system" natural gas grid. This setup is used to assess the physical impacts of HIGG on a pipeline network.

The GRHYD project in Dunkirk, France, which began operating in 2017, has similar objectives but is of a larger scale, injecting hydrogen produced by electrolysis into a gas grid supplying around 200 new homes [66]. The injection blend level will be stepped up to levels of 6 vol.%, 13 vol.% and finally 20 vol.%. The electricity supply rate from the electricity grid will be varied to simulate the effects of a variable renewable supply. Finally, of a similar scope is the planned HyDeploy project at Keele University in the UK. This project will see hydrogen blends of up to 20 vol.% injected into the university's private gas network in order to assess the performance of the network and all of the associated appliances. The university campus contains a variety of gas users including homes and more heavy duty use, so is representative of a town of 12,000 residents. After planning and checks on the network, hydrogen injection is due to take place for one year from April 2019 [72].

HIGG has seen the most development in continental Europe, predominantly Germany. Here, several projects are using electrolysis for electric load balancing, and have shown that electrolysers are capable of rapidly following variable loads, and that low levels of hydrogen (typically not more than 5 vol.%) can be injected with no technical issues. However, these projects are still in the exploratory stages, and many are still attempting to find sustainable business models, with or without government support. The economics of HIGG projects is explored further in Section 2.4.

One of the first projects of this kind was by energy company Thüga in Frankfurt, Germany [54], where grid electricity was used to power a 315 kW PEM electrolyser, and the produced hydrogen was injected into the local 3.5 bar gas distribution grid at a controlled blend level of 2 vol.%. Results from the project showed that the system was quick enough to be able to access the electricity balancing market.

Several projects are still in operation, including two plants from German energy company Uniper: WindGas Falkenhagen [55] and WindGas Hamburg [60]. In Falkenhagen, 2 MW of alkaline electrolysis capacity is connected to a wind farm and the produced hydrogen is injected into the 55 bar gas transmission grid at a blend level of 2 vol.%, showing that hydrogen injection into high pressure pipelines can be achieved, at low levels at least. In the first year of operation, Uniper claim that they injected 2 GWh of hydrogen into the grid. In Hamburg, 1 MW of PEM electrolysis capacity is connected to a wind farm, trialling the newer technology at a larger scale.

Further German projects include one in Hassfurt [65], which includes 1.25 MW of PEM electrolysis capacity and can inject up to 5 vol.% into the gas grid when excess renewable electricity is available, and one in Brunsbüttel [68], with a single 2.4 MW PEM electrolyser connected to a nearby 15 MW wind park. One of the few grid balancing HIGG projects being carried out outside of Germany is the Wind2Hydrogen project in Austria [63], but this is quite small in size with only 100 kW of PEM electrolysis capacity.

Three projects in this category enhance the load balancing offering with CHP in addition to HIGG. The first is the Hybrid Power Plant Enertrag [58], based in Prenzlau, Germany, which can store the hydrogen produced by a 500 kW alkaline electrolyser and use it at a later time in combination with biogas in a CHP unit [39], or alternatively inject the hydrogen directly into the gas grid. In the first three months, 100 MWh of hydrogen were injected. In Solothurn, Switzerland, grid electricity is used in a 350 kW PEM electrolyser, and the resulting hydrogen is stored, and injected into the gas grid [61]. Meanwhile, an on-site CHP unit is operated using gas from the grid. Finally, a similar setup exists at the RWE P2G plant in Ibbenbüren, Germany [62]. At times of high renewable generation, a 150 kW PEM electrolyser produces hydrogen for injection into the natural gas grid. At times of low electricity supply, a CHP unit supplied from the gas grid produces electricity and heat.

The Energiepark project in Mainz, Germany is the largest HIGG project in operation, with electrolysis capacity of 3.75 MW. Electricity input is available from both the grid and a nearby wind farm, and hydrogen is injected into the 6–8 bar gas grid, at blend levels of up to 15 vol.% [59].

There are also several electric load balancing projects that are yet to begin operation. Several of these are based in Germany and are of a similar scale to existing projects, such as the RH2-PTG project [75], the HPEM2GAS project [71], and a project run by EnergieDienst in Wyhlen [77]. Further planned projects of this scale, but outside Germany include the Jupiter 1000 demonstration project [67, 70] in Foss-sur-Mer, France, which will demonstrate P2G, HIGG and MIGG using both PEM and alkaline electrolysers; a project in Ontario, Canada [73], and the first HIGG project in Australia [69].

A larger project, with 6 MW of electrolysis capacity, is planned in Etzel, Germany [76], with the primary focus of investigating salt caverns for hydrogen storage but also including HIGG. Of a completely different scale is the planned H2V Product project in Northern France, which will see the installation of 40 alkaline electrolysers, for a total electrolysis capacity of 100 MW. This plant is still in the early planning stages and is the first part of the ambitious H2V Product project which aims to install several large HIGG plants across France [50, 51].

Finally, two of the identified projects have HIGG capability, but not as the main activity of the plant. Rather, hydrogen is only injected into the gas grid when either the capacity of the usual outlet or storage of the plant is exceeded. These are also both located in Germany, at the Berlin Brandenburg Airport [39, 64] and at the Wolfgang Industrial Park in Hanau [74].

2.4 Economic assessment studies on P2G

Significant interest in P2G has led to many assessments of the economics of P2G being performed. These assessments are concerned with the costs and potential usefulness of P2G in the wider energy system. Table 2.2 summarises the studies, with a focus on gas grid injection, that have been reviewed.

Various approaches were taken to assessing the economic potential of P2G and HIGG, including “case study” assessments, looking at specific business cases, such as a particular plant setup; “levelised cost” assessments of the final product gas (usually hydrogen); and wider system cost assessments.

The studies indicate that it is difficult to find profitable business cases for HIGG. Thomas et al. [10], for example, studied eight different renewable hydrogen case studies for the region of Flanders in Belgium and failed to find any competitive scenarios in 2015; the only competitive scenarios were found for industry and transport (not HIGG)

Table 2.2: Summary of power-to-gas economic assessments

Study Type	Author(s)	Year	Geographical Scope	Timeframe	HIGG	Ref.
Case study	Dickinson et al.	2010	South Australia	2010	Not modelled	[78]
	Scamman et al.	2013	UK	2015 – 2050	$\leq$ 21 vol.%	[17]
	de Joode et al.	2014	Regions within the Netherlands	2014 – 2030	0.02 vol.%; 0.5 vol.%; 100 vol.%	[79]
	Bertuccioli et al.	2014	Europe	2012 & 2030	Unspecified low level	[27]
	Guandalini et al.	2015	Generic European country	2015	Unspecified low level	[80]
	Budny et al.	2015	Plant in Germany	2015	On-site pipe storage	[81]
	FCHJU	2015	Europe	2015 – 2050	Not modelled	[82]
	Thomas et al.	2016	Flanders, Belgium	2015 – 2050	Unspecified low level	[10]
	Sadler et al.	2016	Leeds, UK	2013 – 2029	None	[42]
Levelised cost	Schiebahn et al.	2015	Germany	2015	5 vol.%	[12]
	de Bucy	2016	Generic European country	2016 – 2050	Unspecified low level	[83]
	Parra et al.	2017	Plant in Switzerland	2017	10 vol.%	[84]
System cost	Polman et al.	2003	UK / France / Netherlands	2025	$\leq$ 25 vol.%	[1]
	Ma & Spataru	2015	UK	2015	$\leq$ 50 vol.%	[85]

in 2050. This is largely due to the low value of natural gas in the gas grid compared to the higher price of electricity used to produce the hydrogen. Schiebahn et al. [12], for example, found the levelised cost of hydrogen in the gas grid to be almost four times larger than the current gas price. De Bucy [83] and Parra et al. [84] both calculated similar results for 2015, and predicted that although by 2050 the levelised hydrogen cost would fall, it would still be higher than the gas price.

To find more favourable business cases, studies were required to consider the additional benefits that P2G plants could provide, such as grid balancing services. Scamman et al. [17] found that a 1 MW P2G plant could be profitable in the UK in 2030 if it had access to free excess electricity and demand-side management markets. However, these cases are still challenging due to the limited hours where balancing markets or surplus renewable energy are available. As a result, any cases that do find HIGG to be profitable rely on policy support. For example for the same case, Scamman et al. found that a hydrogen feed-in tariff of £170/MWh would be required for the plant to be profitable in 2015. Similarly, Guandalini et al. [80] found profitable cases when hydrogen feed-in tariffs of €20/MWh and a carbon tax of at least €40/tCO_2 were included.

A further challenge is the technical limitations of hydrogen in the gas grid, for example the low allowable concentration of hydrogen in the blend. The assumptions made regarding this constraint vary widely across the literature, which reflects the uncertainty and variability in regulation around the world. In those studies that used very low restrictions, the capacity or demand available for HIGG was found to be too low to offer a worthwhile market. For example de Joode et al. [79] studied three case studies in the Dutch energy system but only allowed a maximum HIGG level of 0.5 vol.%. Consequently, where there was an alternative to P2G available, such as electricity transmission lines, this was economically preferable. Polman et al. [1] performed an investigation of the technical challenges of hydrogen in the gas grids in the UK, Netherlands and France. It was found that small amounts (up to 3 vol.%) of hydrogen could be injected into the gas grid with little cost or impact, which could provide a small but useful outlet for hydrogen produced from renewable energy. However, the cost effectiveness of higher levels of injection was found to be very poor, with a maximum of a 4% reduction in CO_2 emissions being achieved with a 25 vol.% hydrogen injection level. This poor CO_2 mitigation was due to the overall (average) hydrogen blend level being much lower than the peak, the lower volumetric energy of hydrogen, and the non-zero CO_2 impact of the hydrogen (in this study, the hydrogen was produced from SMR with CCS).

Those studies that considered alternative P2G applications found transport to be a more profitable option than HIGG, such as Schiebahn et al. [12], de Joode et al. [79] and Thomas et al. [10]. This is predominantly due to the considerably higher value of energy in the transport market compared to the gas or electricity markets.

The H21 Leeds City Gate project [42] is not a P2G project, as it considers hydrogen production from SMR in its economic assessment of a switch for the city of Leeds, UK, from natural gas entirely to hydrogen. SMR was chosen due to the very large supply of hydrogen required (6 TWh per year). Nonetheless, the potential of electrolysis for supplementing hydrogen supply was identified in the report. Furthermore, the study is of interest due to its ambitious scope and detailed review of the requirements for the production, distribution and end use of hydrogen. For example, the linepack storage capacity of the gas grid was considered, accounting for the reduced calorific value of hydrogen compared to natural gas. As a result, additional intra-day salt cavern storage was included in the design. Further salt cavern storage was also specified to cover inter-seasonal differences in demand, allowing the SMRs to operate more consistently throughout the year. Overall, the study found that the switchover would cost around £2 billion and would reduce the carbon emissions associated with heating in the city by 73%.

Although these studies evaluate possible business cases and identify challenges that need to be addressed if P2G and HIGG are to be profitable, they are limited in a number of ways. Many of the studies focus on the cost or profitability of a few pre-defined cases without considering the wider system benefits. For example, these studies have limited ability to model the intermittency of renewable energy and the need for storage. Furthermore, as they do not model the physical aspects of P2G and HIGG, these studies assumed that these strategies would be technically feasible. Even those studies that do consider the wider system do not take into account system dynamics, instead performing the evaluation based on a few operating points at most.

2.5 Simulation and optimisation of gas and electricity networks with P2G

In this section, studies using more in-depth mathematical modelling of gas and electricity systems and P2G are reviewed. Various categorisations have been used for these techniques: here, a commonly used distinction (e.g. used by [21, 22, 23]) between *optimisation* and *simulation* models is used.

Optimisation modelling involves defining an "objective function", which quantifies the performance of the system as a function of design and operating variables of the system (which are decision variables). This could be any suitable performance metric, such as cost, efficiency or environmental impact. The solver determines the values of the decision variables that maximise or minimise the objective function, subject to a number of constraints. The constraints can be physical limitations of the technologies, such as the maximum amount of energy that can be stored or the maximum rate of operation of a technology, and also policy constraints such as siting of technologies, emissions targets, investment budgets etc.

Optimisation modelling has been used for many applications, and various techniques have been developed [86]. In linear programming (LP), optimisation variables are continuous, and the model constraints and objective function involve only linear functions of these variables. As a result, LP problems are relatively straightforward to solve. However many real life systems exhibit nonlinear behaviour. If these nonlinearities cannot be approximated linearly it can be necessary to include nonlinear functions in either the objective function or the constraints, resulting in a nonlinear programming (NLP) problem. These problems might have improved representation of the physical system, but are considerably more difficult to solve. Additionally, in some cases, variables may be required to take integer values only (for example an on/off binary decision). The resulting problem will be a Mixed-integer linear programming (MILP) or Mixed-integer nonlinear programming (MINLP) problem, which are also more difficult to solve, as continuous optimisation techniques cannot be used.

There can be a trade-off between realistic representation of the problem and solvability. Many energy systems problems are not suited to linear modelling. For example classical gas network modelling involves nonlinear functions of the pipeline pressures. Meanwhile many energy system decisions are binary, e.g. should a plant be built in a certain location, or not? In this section, several methods for overcoming these challenges will be explored.

Unlike optimisation, simulation involves modelling a single scenario based on a fixed set of inputs. Alternative scenarios can be modelled and compared but no decisions are made by the model. In the context of energy systems, simulation models are often thought of as models which generate "forecasts" of the future evolution of systems [23]. However, simulation can also be used at a greater level of detail, for example to model operation of a gas network [87] or individual power plant [88].

Given that a variety of approaches exist for modelling energy systems, particularly when modelling the interactions between gas and electricity networks, a range of models have been reviewed which include simulation, dispatch optimisation, equilibrium optimisation, and supply chain optimisation. Table 2.3 provides details of the models that were reviewed.

Table 2.3: Details of power-to-gas optimisation models

Study author(s)	Model name & reference	Modelling approach	Spatial representation	Temporal representation	Objective function(s)	Key design decisions	Key operation decisions	Gas grid	Elec. grid	HIGG	MIGG
Dodds et al. [14, 89]	UK MARKAL [90]	LP optimisation	UK represented as 1 region	Yearly/decadal time steps, with (unlinked) time-slicing for shorter variability	Min cost	Penetration of each tech. in each year/decade	Average operation of each tech. type in each year/decade	✓	✓	✓	✓
IEA [91]	TIMES [92]	LP optimisation	Global represented as 1 region	Yearly/decadal time steps, with (unlinked) time-slicing for shorter variability	Min cost	Penetration of each tech. in each year/decade	Average operation of each tech. type in each year/decade	✓	✓	✓	✓
de Joode et al. [79]	OPERA [79]	Optimisation (formulation unknown)	Netherlands represented as 1 region (multiple regions can be modelled)	1 year represented, with (unlinked) time-slicing for hourly variability	Min cost	Penetration of each tech. in each year/decade	Operation of each tech. type in representative time slice	✓	✓	✓	✓
Vandewalle et al. [93]	Unnamed [94]	MILP optimisation	Belgium represented as 1 region	1 year represented with a 15 minute time interval & 3 day rolling horizon	Min operational cost	Number of each generation or P2G tech. to be used in the given year	Operation of each tech. in each time interval	✓	✓		✓
Sveinbjörnsson et al. [95]	SIFRE [96]	MILP optimisation	Danish town represented as 1 region	1 year represented with a 1 hour time interval & 1 week rolling horizon	Min operational cost	Penetration of each tech. type for the given year	Operation of each tech. in each time interval	✓	✓		✓

Table 2.3 *(continued)*: Details of power-to-gas optimisation models

Study author(s)	Model name & reference	Modelling approach	Spatial representation	Temporal representation	Objective function(s)	Key design decisions	Key operation decisions	Gas grid	Elec. grid	HIGG	MIGG
Jentsch et al. [97]	Unnamed [97]	MILP optimisation	Germany represented as 18 zones	Unknown time horizon, with a 1 hour time interval	Min operational cost; Min excess energy	Penetration and spatial distribution of P2G techs.	Operation of each tech. in each time interval		✓		✓
Abeysekera et al. [34]	Unnamed [34]	Newton-node simulation	Generic 12 node gas network	Steady state	n/a	n/a	n/a	✓		✓	✓
Hafsi et al. [98]	Unnamed [98]	Newton-loop simulation	Generic 9 node gas network	Steady state	n/a	n/a	n/a	✓		✓	
Pellgrino et al. [87]	Unnamed [87]	Non-isothermal nodal simulation	Italian region represented with 80 nodes (gas)	Steady state	n/a	n/a	n/a	✓		✓	✓
Tabkhi et al. [99]	Unnamed [99]	NLP optimisation	Generic 3 pipeline network with compressor stations	Steady state	Min fuel consumption; Max transmitted power; Max H_2 injection	None	Network pressures and flow rates	✓		✓	
Devlin et al. [100]	Unnamed [100]	MILP optimisation	GB & Ireland represented with 19 buses (elec.) & ∼40 nodes (gas)	1 year represented with a 1 hour time interval & 1 day rolling horizon	Min operational cost	None	Operation of each tech. in each time interval	✓	✓		
Deane et al. [101]	Unnamed [101]	MILP optimisation	EU represented with 1 bus (elec.) & 1 node (gas) per country	1 year represented with a 1 hour time interval & 1 day rolling horizon	Min operational cost	None	Operation of each tech. in each time interval	✓	✓		

Table 2.3 *(continued)*: Details of power-to-gas optimisation models

Study author(s)	Model name & reference	Modelling approach	Spatial representation	Temporal representation	Objective function(s)	Key design decisions	Key operation decisions	Gas grid	Elec. grid	HIGG	MIGG
Zhang et al. [102]	Unnamed [102]	MILP optimisation (elec.) + Newton-node simulation (gas)	Generic network with 6 buses (elec.) & 76 nodes (gas)	1 month represented with a 1 hour time interval	Min operational cost	None	Operation of each tech. in each time interval	✓	✓		
Zhang et al. [103]	Unnamed [103]	MILP optimisation (elec.) + Newton-node simulation (gas)	Generic network with 118 buses (elec.) & 4 nodes (gas)	20 years represented with a 1 month time interval & 3 load blocks per month	Min net present cost	Whether to build candidate generation or transmission techs.	Operation of each tech. in each time interval	✓	✓		
Zeng et al. [104]	Unnamed [104]	Newton-node simulation	Generic network with 9 buses (elec.) & 7 nodes (gas)	Steady state	n/a	-	-	✓	✓		
Qadrdan et al. [105, 106]	CGEN [107]	MINLP optimisation	GB represented with 16 buses (elec.) & 47 nodes (gas)	Up to 1 week represented with a 1 hour time interval & 1 day rolling horizon	Min operational cost; Min total costs	Installed capacity of P2G facilities at different locations	Operation of each tech. in each time interval; transport flows; storage	✓	✓		✓

Table 2.3 *(continued)*: Details of power-to-gas optimisation models

Study author(s)	Model name & reference	Modelling approach	Spatial representation	Temporal representation	Objective function(s)	Key design decisions	Key operation decisions	Gas grid	Elec. grid	HIGG	MIGG
Clegg & Mancarella [3, 108]	Unnamed [108]	NLP optimisation (elec.) + Nodal simulation (gas)	GB represented with 29 buses (elec.) & 79 nodes (gas)	1 year represented with a 30 minute time interval	Min operational cost + Max P2G integration (2-stage optimisation)	Installed capacity of P2G facilities at different locations	Operation of each tech. in each time interval	✓	✓	✓	
Pudjianto et al. [109]	Unnamed [109]	MILP optimisation	GB represented as 5 zones (each with 10 subregions)	1 year represented with a 1 hour time interval	Min net present cost	Whether to reinforce existing infrastructure & invest in candidate infrastructures	Operation of each tech. in each time interval	✓	✓	✓	✓
Geidl et al. [110, 111]	Energy Hub Model [110]	MINLP optimisation	Single plant (”Energy hub”)	1 or more steady state time intervals	Min cost	Configuration of conversion & storage technologies for a given plant	Operation of techs. within plant		✓		
Almansoori & Shah [112, 113, 114]	Unnamed [112]	MILP optimisation	GB represented as 34 zones	6 year time steps, cannot capture shorter dynamics	Min net present cost	Number, size & location of production, transport & storage techs.	Operation of each tech. in each time interval	✓	✓		

Table 2.3 *(continued)*: Details of power-to-gas optimisation models

Study author(s)	Model name & reference	Modelling approach	Spatial representation	Temporal representation	Objective function(s)	Key design decisions	Key operation decisions	Gas grid	Elec. grid	HIGG	MIGG
Mesfun et al. [115]	BeWhere [115]	MILP optimisation	Alpine Europe represented with 3000 grid cells	1 year represented, with (unlinked) time-slicing for hourly variability	Min total cost; Min CO_2 emissions	Number, size & location of conversion techs.	Operation of each tech. in each time interval		✓		✓
Kötter et al. [116]	Unnamed [116]	Optimisation (formulation unknown)	Small region in Germany represented with 17 subregions	Unknown time horizon, with 15 minute time interval	Min total cost	Penetration of each tech. type	Operation of each tech. in each time interval	✓	✓		✓
Samsatli et al. [117, 118, 119, 120]	Value Web Model [119]	MILP optimisation	GB represented as 16 zones	Decadal timesteps for planning and (linked) time-slicing for hourly variability	Min net present cost (or max NPV); Min CO_2 emissions; Max energy production	Number, size & location of conversion, transport & storage techs.	Operation of each tech. in each time interval	✓	✓		✓

2.5.1 Modelling objectives and approach

Simulation models can be used to assess the behaviour of gas in pipeline networks by calculating pressures, flow rates and temperatures under different operating conditions. Several studies have used these techniques to assess the effects of HIGG on pipeline networks, with varying assumptions concerning steady state or transient conditions, compressibility, and isothermal behaviour [87, 34, 98]. These studies use nonlinear gas flow equations to express the pressure drop along a pipeline in terms of the gas properties and the pipe's physical characteristics. Kirchoff's laws are then used to assess gas flow around the network, by ensuring that either nodal gas flows or pressure drops around a loop sum to zero. Zeng et al. [104] used a similar approach, also including an electricity network in the problem: all gas and electricity flows were converted to a per-unit system and were summed to zero at each node.

Whilst simulation models are able to assess the effects of P2G and compare scenarios, they are not able to make decisions. Tabkhi et al. [99] integrated optimisation into a gas network simulation problem by including compressor stations with variable operating regimes. An NLP optimisation was used to optimise compressor performance or energy throughput subject to constraints on the required level of HIGG.

In electrical power engineering, optimisation is widely used to solve the Optimal Power Flow (OPF) problem. In its classic form, the OPF is a combination of the economic dispatch problem with electricity network power flow equations [121]. The cost of generation is minimised for a point in time, based on the generators available on the network (each of which has its own operation cost curve), subject to network power flow constraints. The cost curves are often nonlinear, leading to the additional challenges of solving an NLP problem. Various versions of the OPF problem exist, such as scheduling and planning problems which have longer time frames and often include binary on/off decisions – resulting in a MINLP (or sometimes MILP) problem. Jentsch et al. [97] and Kötter et al. [116] both used OPF models to assess the potential for P2G in high renewable energy scenarios, but each used simplifications to maintain linear problems.

Clegg and Mancarella [3, 108] combined a gas network simulation with an OPF model. A two-stage optimisation was used: first, the OPF problem was solved for an electricity network. Then, an optimisation was performed to install P2G facilities in the locations which would provide the maximum benefit, in terms of the unused renewable power generation available from the first dispatch. Finally, a gas network simulation was performed to balance gas supplies (including from P2G) with demands (including from electricity generators). A transient gas flow analysis was performed in [108], whilst a steady state analysis was performed in [3]. In both cases, a nodal balance was performed to ensure that the optimal electricity dispatch could be supported by the gas network. If a solution could not be found, the two-stage optimisation could be re-run with additional constraints at the gas nodes which could not be solved. A similar approach was used by Zhang et al. [102]. Whilst this approach is able to find a cost optimal electricity dispatch which maximises the benefit of P2G and is feasible for the gas network, the solution might not be optimal for the overall system as dispatch and P2G are optimised separately, and gas network operating costs are not taken into account.

OPF was also combined with gas network modelling in the CGEN model, developed by Chaudry and co-workers [107]. In this case the gas network nodal balance constraints were included in the optimisation at every timestep, which helps to ensure that the solution is optimal for the whole system. Devlin et al. [100] and Deane et al. [101] also developed models which perform OPF and gas flow balancing at every timestep. In order to retain a linear (MILP) problem, linear generator cost curves were used and the gas flow was modelled as "energy flow", rather than modelling pressures around the network.

"Equilibrium" models assess the wider energy system by taking into account economics and resource supplies and demands. Objective functions can include operational and investment costs in order to seek an overall optimum system design. Whilst they are often able to consider a large number of different technologies, these models can lack the resolution to model finer details. For example, they might only consider overall penetration of a given technology type, rather than installation of specific facilities. As a result, many equilibrium models exclude integer decisions altogether.

Most well known and widely used in this category is the MARKAL/TIMES family of models [92, 122]. Dodds and McDowall [89] used the UK MARKAL model to assess the potential for HIGG in the UK, whilst the IEA used TIMES to assess P2G in their Hydrogen and Fuel Cells Technology Roadmap [91]. Other equilibrium models that have been used to assess P2G include the OPERA model [79], SIFRE [96], and the model used by Vandewalle et al. [93, 94].

A final category is supply chain models. Traditionally, supply chain models were developed to optimise the operations (and sometimes the design) of manufacturing supply chains, which may include demand forecasting, logistics, inventory management, taking account of production and delivery lead times. Supply chain models have been applied to energy systems, and can be used to optimise system design, such as types, sizes and locations of energy conversion, transport and storage technologies, whilst accounting for the operation of these technologies in different timesteps. Typically these models involve discrete decisions regarding whether technologies are installed, and form MILP problems as a result.

Almansoori and Shah [112, 113, 114] developed a hydrogen supply chain model concerning the production and distribution of hydrogen for mobility, however the gas and electricity grids were not included. Other notable supply chain models which have included the gas and electricity grids are the BeWhere model, developed by Mesfun et al. [115], and the Value Web Model, developed by Samsatli and co-workers [119].

2.5.2 Modelling of gas-electricity interface

In practice, there are different ways in which energy can be transferred between the gas and electricity networks. Gas-to-power conversions (such as combined cycle gas turbines) are the conventional interface, and many studies, such as Devlin et al. [100], Deane et al. [101], Zhang et al. [102, 103], and Chaudry and co-workers [107, 123, 124, 125, 126], only included these.

Power-to-gas conversions include HIGG and MIGG. Several studies included MIGG, such as Vandewalle et al. [93], Sveinbjörnsson et al. [95], Zeng et al. [104], Mesfun et al. [115] and Kötter et al. [116]. The MIGG interaction is fairly simple to model. Assuming that the impacts of MIGG on the behaviour of the gas grid are minimal, it can be represented by a conversion efficiency between a quantity of electricity and a quantity of gas. As Jentsch et al. [97] did not model gas flows, MIGG was only modelled as a revenue from selling the produced methane at the gas price.

Due to the differing physical properties of hydrogen compared to natural gas, the behaviour of hydrogen in the gas grid is more complex. Those studies which have modelled HIGG have taken a range of approaches to modelling these effects.

Dodds et al. [89], IEA [91] and de Joode et al. [79] only considered overall demands and supplies of energy, so only the efficiency with which hydrogen can be produced (e.g. from electricity) was considered. Qadrdan et al. [105, 106] converted injected hydrogen into the equivalent volume of natural gas which would carry the same quantity of energy, effectively modelling HIGG in the same way as MIGG. In this way, energy flows are represented but the volume of gas in the network is underestimated and pressure effects are not accounted for.

An alternative method assumes that the blend level of hydrogen is uniform throughout the grid. Hence, the average calorific value of the gas in the grid is reduced according to the overall proportion of hydrogen injected compared to natural gas. In this way, energy and volumetric flows, and hence also pressure effects, are appropriately modelled. This approach was adopted by Hafsi et al. [98], Tabkhi et al. [99], and Clegg and Mancarella [3, 108].

Finally, Pellegrino et al. [87] and Abeysekera et al. [34] tracked varying gas compositions due to hydrogen injection throughout the network by ensuring that both volumetric and mass flows were balanced at each node. This is particularly relevant where hydrogen injection occurs at distributed locations, as is the case in these studies, and is likely to be the case in real-life HIGG scenarios.

2.5.3 Storage and linepack

Gas grids have an inherent flexibility, known as linepack, because the volume of the pipework itself is treated as a storage vessel. Assuming that the network may be operated within a defined range of pressures, the quantity of gas stored within the pipework can be varied. Gas network operators exploit this behaviour to allow for some flexibility between gas supply and demand. Typically, it is ensured that enough gas is supplied to the network to meet demand on a daily basis, but during the day the linepack can vary [127]. When modelling P2G and gas grid injection, it is important that this flexibility is represented appropriately.

Several models included representation of the gas grid for transport, but did not include any grid flexibility, so gas grid supplies and demands needed to be balanced at each timestep (e.g. hourly). Nonetheless many of these models did include gas or hydrogen storage as either pressurised vessels or underground storage, enabling some overall flexibility. Examples of these models include the model used by Deane et al. [101], the model used by Sveinbjörnsson et al., the Value Web Model [119] and OPERA [79]. Meanwhile Mesfun et al. [115] and Kötter et al. [116] both represented the gas grid as an infinite storage resource: methane could be injected into or withdrawn from the grid without any consideration of the overall supply of gas.

Several studies which modelled gas network pressures were able to model linepack. In Devlin et al. [100], Zhang et al. [102] and Zeng et al. [104], linepack was modelled by using constraints to define allowable network pressure ranges. In Qadrdan et al. [106] the linepack was directly calculated based on pressures and pipe volumes, tracked between timesteps, and constrained. Clegg and Mancarella [3, 108] used a similar approach, but the gas flows were only solved on a daily basis, which added some additional intra-day flexibility and is representative of the way in which systems operators manage linepack.

In order to fully capture the flexibility of the gas network it is important that linepack is modelled. However, modelling all of the gas network pressures is computationally demanding and nonlinear. Vandewalle et al. [93] is the only study that has been identified that modelled linepack flexibility without modelling gas network pressures. Instead, for each timestep a gas flexibility variable was included so that supplies and demands do not have to match exactly. The flexibility variable was unconstrained in each timestep, but was made to sum to zero in each twenty-four hour period (so that any deficits and surpluses balance over one day). Additionally there was a cost which scaled linearly with the range of flexibility demanded within one day, representative of any costs which may be incurred by the system operator in managing this flexibility.

2.5.4 Spatio-temporal representation

Details of the spatio-temporal representations in the models that have been reviewed are given in Table 2.3.

The majority of the models include a spatial resolution, either representing a geographic region as a series of interconnected zones (e.g. in the Value Web Model [119]), or as a series of nodes which represent important locations in the gas or electricity infrastructure (e.g. in the CGEN model [107]). However, the more high level equilibrium optimisation models, such as MARKAL/TIMES [92, 122], OPERA [79] and SIFRE [96], lump the region they are representing as one, with no spatial representation. Consequently these models cannot accurately model the costs or practicalities of the transportation of energy. In Dodds and McDowall [89], for example, the value of the UK gas grid was assessed despite having no representation of spatial transmission and distribution requirements.

When modelling P2G and the influence of intermittent renewable energy, high temporal resolution is required to capture the short term balancing needs between supply and demand. Meanwhile, it can be important to optimise over long enough time horizons to ensure that, for example, network operation is optimised for interseasonal variabilities, and even investments in network design are optimised at decadal timescales.

Some models are able represent high temporal resolution with contiguous timesteps of around one hour. This captures the short term dynamics very accurately, however due to computational demands, only short time horizons (typically a number of days) can be optimised. A commonly adopted solution for modelling longer time periods is a rolling time horizon, where a relatively short horizon of between one day and one week is optimised at a time. The final conditions of one time horizon can be used as the starting conditions of the next horizon. This approach was used by several studies including Vandewalle et al. [93], Sveinbjörnsson et al. [95] and Qadrdan et al. [105, 106]. In this manner, longer periods of time are modelled without requiring an optimisation of a very large number of timesteps at once. It can also be argued that a rolling horizon is representative of the lack of reliable longer term forecasts of supplies and demands. However an overall optimum for the entire time horizon is not found: for example, interseasonal storage would not be optimised. Furthermore, despite its simplifications the rolling horizon approach is still relatively computationally demanding.

An alternative approach is to use time-slicing, where a small number of time intervals are selected to represent typical system behaviour. For example, a day could be split into periods of low, medium and high demand, or one representative day could be chosen for each season. When these time-slices are optimised they can be repeated and combined in order to develop a complete representation of a year or more of operation. In MARKAL/TIMES [92, 122], OPERA [79] and in Mesfun et al. [115] time-slicing is used, however each time slice is optimised in "steady state", with no linking between intervals. As a result, although the computational demand is low, system dynamics, for example for storage, are not modelled. The Value Web Model [119] overcomes this by allowing changes (such as storage inventories) to occur over the course of the time interval, using constraints to manage the conditions at the start and end of a series of repeated intervals. This approach is more computationally demanding than unlinked time-slicing, but allows for a considerably better representation of system dynamics on both a short term (such as hourly) and medium term (such as interseasonal) scale.

Finally, it is desirable to be able to model longer time periods, such as years or decades, in order to carry out system planning and investments. For example, the MARKAL/TIMES models [92, 122] have yearly or decadal timesteps for investment decisions. In their supply chain planning model, Almansoori and Shah used 6-year time periods over a time horizon of up to 30 years [113]. Zhang et al. adjusted their short-term operation optimisation model so that it could be used for infrastructure planning, by increasing the timestep from hourly to monthly [103]. Using the linked time-slicing technique, the Value Web Model [119] is capable of capturing both short term variability and long term planning. Yearly or decadal time intervals can be used in order to make planning decisions. However, computational tractability becomes a significant challenge for any model that simultaneously considers such a range of time intervals.

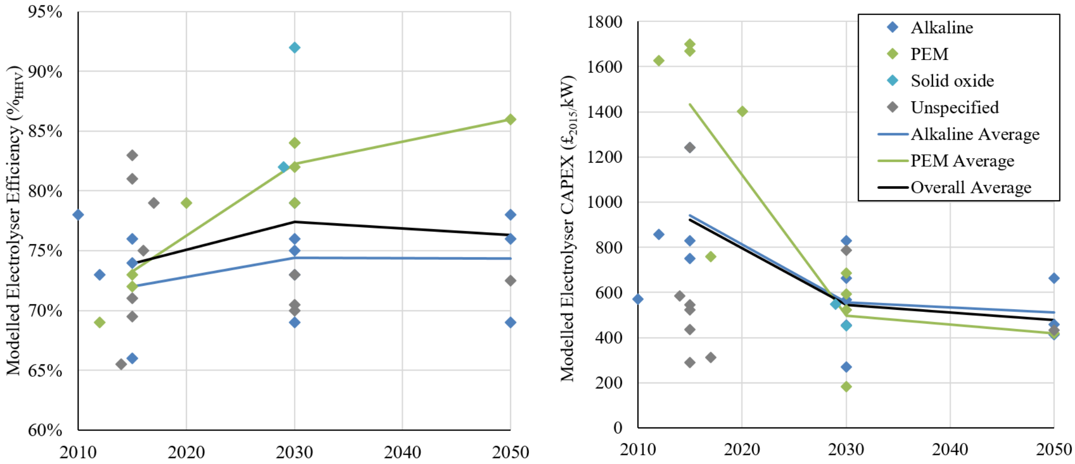
2.6 Comparison of scope, assumptions and outcomes of models and real-life projects

All of the real life projects, economic studies and optimisation studies that have been reviewed are concerned with using P2G and HIGG for either grid balancing or decarbonisation of heat. Many real-life projects and economic studies assessed the potential of HIGG for grid balancing from the plant operator perspective, for example investigating whether it is feasible to use HIGG in conjunction with a wind farm. Typically, these economic studies represent scenarios realistic to the real-life projects: Thomas et al. [10], for instance, used information directly from the Uniper HIGG project in Falkenhagen [55] in their economic study. Alternatively, the potential for HIGG from a system wide perspective was assessed. Several real-life projects are investigating the practicalities of HIGG for higher injection levels. Some economic studies have also attempted to take a whole-system perspective; however, optimisation studies are best suited to this as they can model the operation of the system and make operational and investment decisions. However, to date, relatively few optimisation studies have included HIGG.

Regarding input data assumptions, two key parameters are electrolyser efficiency and electrolyser cost. Figure 2-7(a) shows the electrolyser efficiencies that were assumed across all the modelling based assessments, based on the higher heating value of the hydrogen produced divided by the electricity input ($\%_{\mathrm{HHV}}$). Although the range over all electrolyser types is large, agreement for a given technology type is fairly good, and all studies predict improvements in efficiencies by 2030.

An equivalent plot for electrolyser capital expenditure (CAPEX) is shown in Figure 2-7(b). There is a wide range in assumed CAPEX in 2015, but this can again be explained by differing technology types: PEM electrolysers are agreed to be more expensive in 2015. Costs are expected to fall by 2030 for both of the main technologies, more so for PEM. Nonetheless, in 2030 there is a range of £646/kW in the assumed electrolyser CAPEX. The effect of electrolyser CAPEX on project profitability is unclear: Kötter et al. [128] found the impact of electrolyser CAPEX to be small, however the falling cost of electrolysers between now and 2030 was enough for Scamman et al. [17] to conclude that projects that are not profitable today will be profitable by 2030.

The assumed electrolyser plant size varied from less than a megawatt to hundreds of megawatts, so assumptions regarding economies of scale are also important. Meanwhile a variety of measures have been modelled, such as negative electricity prices, carbon prices and "green" hydrogen tariffs. Determining realistic and probable future business



(a) (b)

Figure 2-7: **Input data assumptions in all economic and optimisation studies:** (a) electrolyser efficiencies ($\%_{\mathrm{HHV}}$); and (b) electrolyser CAPEX ($£_{2015}$/kW). References for the studies are provided in Tables 2.2 and 2.3.

models will be important for any future modelling.

Figure 2-8 shows the maximum levels of hydrogen injection allowed in the real-life projects, in addition to the assumed maximum injection level in the modelling studies. The assumed level in the modelling studies varies widely. Many studies considered multiple discrete maximum injection levels, up to 20 vol.% or even higher, which seems appropriate based on the real-life projects such as the Ameland project that have shown that blends at around this level can be achieved. Those studies, such as Schiebahn et al. and de Joode et al., and indeed the real-life grid balancing projects, that allow much lower levels of hydrogen injection are arguably overly pessimistic. Many of the studies that are shown in Figure 2-8 to have investigated 100 vol.% injection levels modelled this as an independent "pure hydrogen" case, rather than modelling an unconstrained level of injection up to a maximum of 100 vol.%.

Whilst local, practical issues with higher levels of HIGG have been shown to be minimal, wider effects such as energy delivery and management of linepack are currently less certain. Modelling can be used to understand these uncertainties, and operational studies that have been performed conclude that issues with pressures and throughput should be manageable.

Regarding further results and conclusions of the real life projects and modelling, it is clear that in the current economic and policy landscape it is challenging to find profitable business cases for HIGG. Economic studies used a variety of policy support

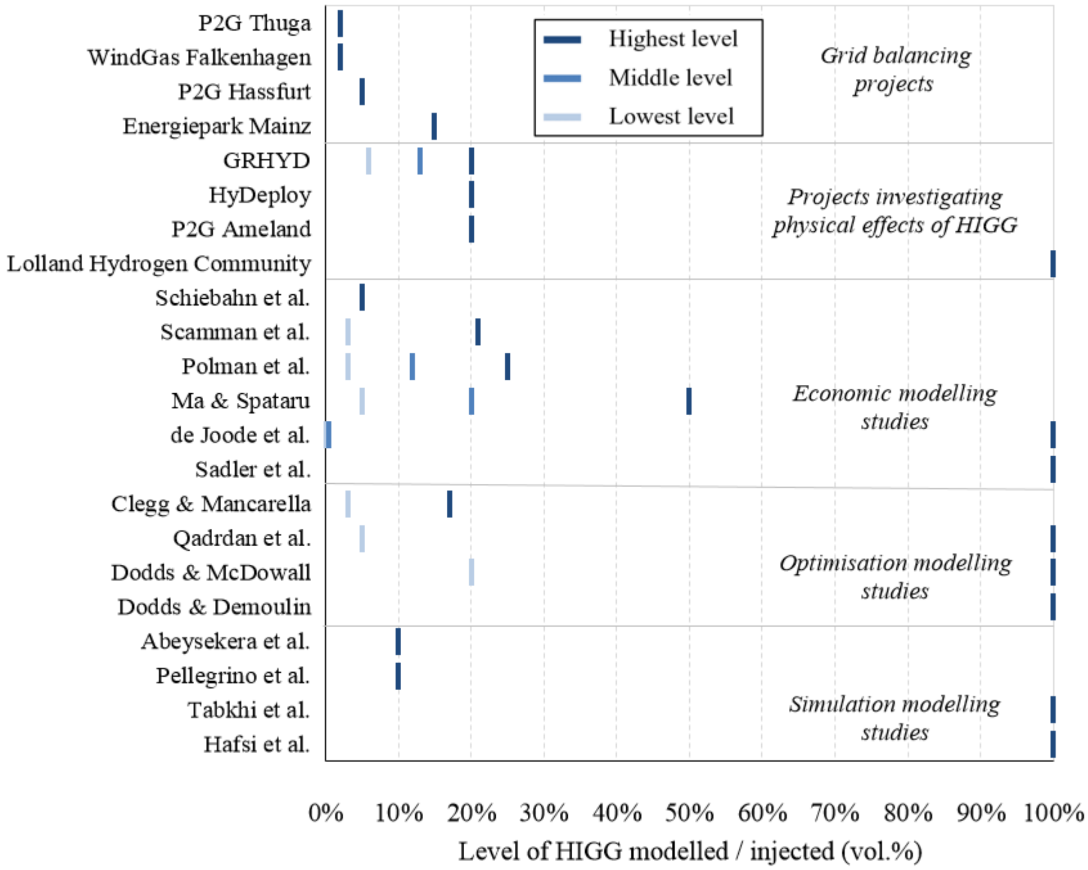


Figure 2-8: **Maximum levels of hydrogen injection used in real-life projects and assumed in modelling studies.** Where a project/study investigated more than one discrete injection level, this is shown using the “lowest”, “middle” and “highest” level markers. References for the projects and studies are provided in Tables 2.1–2.3.

measures to find profitable business cases, whilst real life projects are yet to reach commercial scale. A variety of scenarios were considered in the modelling scenarios, but all identified the potential for P2G to help increase penetration of renewable energy into the energy system. Many of the modelling studies predict more profitable pathways for hydrogen as a transport fuel, due to the higher value of energy when used in transport. This result is supported by the large number of P2G projects which deliver hydrogen for transport.

2.7 Conclusions

From the number of real life P2G projects and economic and optimisation studies including gas grid injection it is clear that there is considerable interest in this area. However, there are challenges: HIGG projects that have been carried out are yet to reach commercial scale, and economic studies have indicated that, whilst profitable business cases may be possible, they will require complex scenarios such as electricity balancing markets or government support through taxes or subsidies. Additionally, there are technical challenges such as the physical issues with mixing hydrogen with natural gas and maintaining a stable overall system. Further real life testing will help to identify and understand the physical challenges of individual technologies, whilst modelling will play an important role in evaluating the system effects. Despite the challenges for P2G, the overall outlook from the literature is positive, although some contributors such as electrolyser manufacturers may arguably have an interest in magnifying the potential of P2G.

Whilst the field of optimisation modelling for energy systems is vast, P2G has only just begun to be considered. P2G is incorporated into some high-level system models such as MARKAL/TIMES, but these lack the spatial and temporal resolution to model appropriately the business cases that are being identified for P2G. Various studies have investigated the physical impact of HIGG on the gas and electricity grids, and this work is highly useful for establishing what the challenges will be for systems operation and how to overcome them. However, with such a close focus on the operational details of the networks, these models lack a view of the wider picture, and so are unable to represent system issues such as interseasonal variability and CO_2 emissions.

A class of optimisation models exist which are capable of capturing these wider system issues, as well as the fine spatio-temporal resolution needed to represent variability and operational issues. However, although some of these models have included hydrogen as an energy vector, perhaps for transport, none have modelled the intricacies of P2G and

HIGG, such as linepack storage, grid upgrades and the effect of hydrogen blends on end-use. These models should be developed in order to incorporate P2G and HIGG, using results from the real-life projects, economic studies and operational network models to guide the scenarios that are modelled.

Small advances in the technologies involved in P2G are taking place, and efficiencies and costs are expected to improve by 2030. However, these improvements are unlikely to be dramatic enough to make significant differences to business cases, unless a currently little-known technology makes strong progress and becomes a game-changer, such as reversible solid oxide technology. However, with further operating experience, and increased understanding from modelling, real-life projects will be able to discover the most viable business models. The economic landscape is likely to become more appealing, as systems operators value flexibility more highly, and will be more likely to reward flexibility providers such as P2G plants.

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Chapter concluding remarks

In the concluding remarks for this chapter, the findings of the review article are discussed in the wider context of the thesis, and some minor clarifications (identified since the article was published) are detailed. Finally, a brief update is provided on the developments for real-life power-to-gas projects since the review was published. These concluding remarks have their own reference list at the end of the chapter.

Implications for the thesis

The article that has been presented in this chapter is a valuable review for the thesis, establishing the current technological and research landscape for power-to-gas and gas grid injection. Some specific findings that will be particularly useful for the rest of the project are outlined the following paragraphs.

Firstly, the review found a strong and rapidly growing interest in hydrogen and power-to-gas, from private companies, governments and researchers. Furthermore, the review shows that there are issues concerning hydrogen and power-to-gas that could be better understood, such as the practicalities of injecting hydrogen into gas grids, how power-to-gas and gas grid injection should be deployed, and what the optimal economic cases are. A further (and more up-to-date) discussion of these practical issues is provided in Chapter 5 of this thesis. The growing interest in power-to-gas and need for further research that have been identified provide justification for the thesis topic.

The review also gathered valuable information that will inform the modelling work of the thesis. From the methods and results of the various modelling studies, as well as experience from real-life projects, some key requirements can be determined for a model to accurately represent hydrogen supply chains in the context of power-to-gas, gas grids and the wider energy system.

First, it is important that suitably high spatio-temporal detail is included in the model. This is so that the valuable energy system flexibility services that hydrogen may be able to provide are accurately modelled. In fact, several studies that were reviewed suggested that these flexibility services may be essential for hydrogen technologies to be profitable.

Next, it is important that the electricity and gas transmission and distribution networks are modelled accurately, including any interfacing between the electricity and gas systems. This is so that the valuable functions that these networks provide, and the potential for hydrogen and power-to-gas to augment the operation of these networks, is represented. For example, the opportunity to use power-to-gas to harness some of the flexibility of the gas system to benefit the electricity system could be valuable, but has not been studied in detail.

Finally, the review acquired valuable data that can be used to determine the input data for future modelling work. The acquired data includes technology cost and performance data, from both the real-life projects and the modelling studies. The economic and policy assumptions made by modelling studies, such as electricity costs, levels of feed-in tariff, and CO_2 prices are also useful. Finally, the results from the other modelling studies can also be used to help to validate the results of future modelling work.

Article clarifications

The following clarifications have been identified since the article presented in this chapter was published:

- In section 2.2.1, both the processes of steam methane reforming (SMR) and CO_2 methanation are discussed. It should be noted that SMR is essentially the reverse reaction to CO_2 methanation.
- In Figure 2-1, H_2O should also be included as an input to SMR (in addition to CH_4). Additionally, the figure caption should refer to “CO_2 methanation” rather than “methanation of hydrogen”.

Update to review of real-life projects

Given that the review article presented in this chapter was published in 2018, it is valuable to provide an update on developments since then in the field of power-to-gas. As the review article has shown, there is considerable interest in power-to-gas, with both the number and size of new power-to-gas projects growing each year. Meanwhile, the detailed review of gas grid injection projects can also be updated by considering the progress of those projects, and detailing any new projects that have been announced.

Growth in power-to-gas

The growth in the number and size of new power-to-gas projects that was identified in the review article has continued. In September 2019, the International Renewable

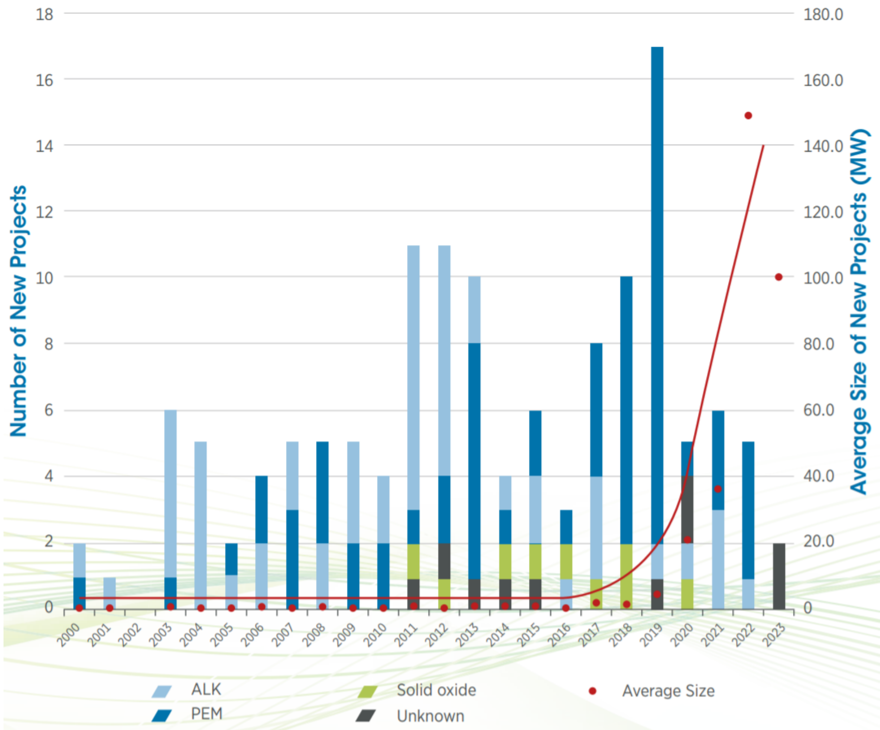

Figure 2-9: Updated timeline of power-to-gas projects going into operation. Reproduced from [1], in which the results in Figure 2-3 were updated with projects from the IRENA database.

Energy Agency (IRENA) published a report considering the potential of hydrogen in the context of renewable energy [1]. As part of this report, IRENA used the review article that is presented in this chapter, and updated it with data from the IRENA database. The main result from this, an updated version of Figure 2-3, is shown in Figure 2-9.

As Figure 2-9 shows, the IRENA study confirmed a continuation of the growth in new power-to-gas projects. As with Figure 2-3, the reduction in numbers of new projects after 2019 is likely to be due to a lack of data, rather than an actual reduction in projects.

The IRENA study identified a large number of new power-to-gas projects either deployed or announced since the original review article was published. The study found that Germany continues to take the lead with power-to-gas: in particular, the German government approved 11 new power-to-gas demonstration projects in July 2019 [1]. Nonetheless, many other countries are also showing continued interest in power-to-gas, including the Netherlands, Norway, Japan, Australia, France, UK, Canada, USA and China [1].

The most significant observation from Figure 2-9 is the rapid growth in project size. According to IRENA, the average project size will exceed 100 MW by 2022, compared to average sizes before 2020 of less than 5 MW. Almost all of the new projects detailed in the IRENA study are at least 10 MW in size, whilst in the original 2018 review, only one project larger than 10 MW was identified: the H2V Product project in France [1, 2].

Another interesting finding in the IRENA report is an increased focus on industrial applications for power-to-gas projects. In the original review, only 12% of projects included "industry" as an application (14 out of 111 projects where the application was specified). The more popular applications were transport, power and gas grid injection (see Figure 2-6). However, in the IRENA study, 58% of the new projects that were identified included industry as an application (14 out of the 24 new projects that were not included in the original 2018 review). Applications for these projects include refining, synthetic fuels and chemical production [1].

A number of large, new power-to-gas projects have been announced even since the IRENA review was published in September 2019, which indicates the continued interest and growth in the area. For example in China, construction has started on a large hydrogen facility to be powered by solar power; the facility will consist of two electrolysis plants, each with a hydrogen capacity of 30 MW (based on lower heating value (LHV)) [3]. In Australia, an electrolysis plant with a hydrogen capacity of 35 MW (LHV) has received funding for the first stage of construction [4]. Larger projects have also been announced that are still at the feasibility stage. For example in the UK, a consortium have received funding from the UK government to carry out a Front End Engineering Design (FEED) study on a 100 MW (nominal) system to supply a refinery [5]. Meanwhile a Chinese electricity generator has signalled that it intends to build a very large wind, solar and hydrogen facility with a hydrogen capacity in excess of 1500 MW (LHV) [6].

Power-to-gas for the gas grid

As has been described, the largest growth area for power-to-gas since the review article was published in 2018 has been for industrial uses of hydrogen. However, there have also been developments in the field of power-to-gas for gas grid injection, including progress in the projects that were included in the review article, and announcements of new projects.

Several of the early-stage projects from the detailed review of hydrogen injection (sec-

Table 2.4: Details of new hydrogen injection projects announced since the original review.

Project	Country	Status	Hydrogen production	Hydrogen injection	Ref.
Contursi	Italy	Operational	Unknown	10 vol.%	[11]
Hydrogen Park South Australia	Australia	Commissioning	1.25 MW electrolysis	5 vol.%	[12]
HyDeploy North East	UK	Commissioning	Electrolysis (unknown size)	20 vol.%	[13]
Schopsdorf	Germany	Unknown	Unknown	20 vol.%	[14]
Element One	Germany	Planning	100 MW electrolysis	2 vol.%	[15]
Hybridge	Germany	Planning	100 MW electrolysis	100 vol.%	[16]
Get H2	Germany	Planning	Electrolysis (unknown size)	100 vol.%	[17]
HyOffWind	Belgium	Planning	25 MW electrolysis	Unknown	[18]

tion 2.3.2) have reported progress since the review was published. The UK project HyDeploy compiled a large safety case to justify the injection of up to 20 vol.% hydrogen into the private gas network, and began injecting hydrogen at the beginning of 2020 [7]. Meanwhile, GRHYD, a French project with a similar scope to HyDeploy, is nearing the end of its main injection trial, having succeeded in injecting hydrogen at fixed levels of 6 vol.%, 10 vol.% and 20 vol.%, and is now operating the electrolyser variably, only generating hydrogen when "green" electricity is available [8]. The HPEM2Gas project also successfully demonstrated the operation of a 200 kW electrolyser and injection of the hydrogen into the local gas grid at 8.5 bar [9]. Finally, the Jupiter 1000 project has completed construction and began injection in February 2020 [10].

Since the review was published, several new hydrogen injection projects have been announced or even begun operation. Details of some of these projects are shown in Table 2.4.

Since the original review, a trial injecting hydrogen into a portion of gas grid supplying two industrial users in Italy has started, and the injection level was recently raised to 10 vol.% [11]. Meanwhile, several new projects have been announced that plan to inject hydrogen into gas grids in the near future. In Australia, a hydrogen injection trial similar to the HyDeploy and GRHYD projects is currently being commissioned, in which hydrogen will initially be injected at 5 vol.% into the local gas grid [12]. A second phase of the HyDeploy project is currently in preparation, in which hydrogen will be injected into a region of the public gas grid at up to 20 vol.% [13]; a similar project has also been announced in Schopsdorf, Germany [14].

Several other projects involving hydrogen injection into gas grids are also being discussed, but are mostly still at the planning stage. Notable projects include the Element One project in Germany, which intends to convert electricity from North Sea wind farms to hydrogen, to be used in various applications including injection into gas grids at up to 2 vol.% [15]. In the Hybridge project, also in Germany, some existing natural gas pipelines will be completely converted to hydrogen to supply industry, whilst partial injection will also be carried out for other users [16]. The Get H2 project has a similar plan, but also has ambitions for a national hydrogen transmission system in Germany, consisting of new hydrogen pipelines and re-purposed natural gas pipelines, and connecting various industrial users across the country [17]. Finally, in Belgium, a hydrogen project is being planned that will include various applications including hydrogen injection [18].

Conclusion

The growing interest in power-to-gas that was identified in the original review has clearly continued in the last two years. The most significant development in this time is the scale-up in ambition for electrolysis plant size, with plant sizes in excess of 100 MW now being planned. Although projects of this scale are still at the planning stage, they show the significant global interest in power-to-gas. Electrolyser roll-out at this scale would also help to achieve cost reductions through learning and economies of scale, potentially leading to reduced hydrogen costs. The increased interest in power-to-gas for industrial applications may have arisen from increased decarbonisation ambition (e.g. "net-zero" emissions targets), which has forced the sector to put new effort into decarbonisation.

Progress in hydrogen injection into gas grids that supply homes has been steady since the review article was published: most projects in this category are still establishing the confidence that more widespread use of hydrogen in homes is safe and practical. However, as with power-to-gas projects more widely, there is an accelerating interest in hydrogen injection for industrial applications. All of the larger hydrogen injection projects that are shown in Table 2.4 are focussed on industrial applications. There may be advantages to focussing hydrogen injection on industrial applications, as they could represent a larger hydrogen demand in a focussed location, thus reducing the extent of distribution network and end-users that would need to be converted or upgraded.

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Chapter 3

Perspective: The need for adequate scenarios and models to represent hydrogen

Chapter introductory remarks

This chapter is based on the perspective article published by the Royal Society of Chemistry in Sustainable Energy and Fuels. The article was published as open access, meaning that material from the article can be reproduced provided that correct acknowledgement is given. The original article reference is as follows:

> Christopher J. Quarton, Olfa Tlili, Lara Welder, Christine Mansilla, Herib Blanco, Heidi Heinrichs, Jonathan Leaver, Nouri J. Samsatli, Paul Lucchese, Martin Robinius, and Sheila Samsatli. The curious case of the conflicting roles of hydrogen in global energy scenarios. *Sustainable Energy and Fuels*, 4:80-95, 2020. https://doi.org/10.1039/C9SE00833K

The article is a perspective, written in collaboration with researchers from various organisations, under the framework of Task 38 of the International Energy Agency Hydrogen Implementing Agreement (IEA HIA). The ideas for the paper were formed at a workshop, held at the University of Bath in June 2017, at which the challenges for modelling hydrogen within energy systems were discussed. At the workshop it was agreed to write an article in order to develop and publish the ideas that were discussed.

As the lead author of the article, I made a significant contribution to the development of the ideas, the structuring of the arguments, and the final presentation of the article. Furthermore, the content of the article is highly relevant to this thesis.

The perspective starts with an overview of the many possible applications of hydrogen in energy systems. The main contribution of the article is an analysis of the most influential global energy scenarios, as well as providing a critical discussion of the results and methods of a selection of smaller studies.

Finally, the perspective develops some clear arguments regarding the requirements for modelling hydrogen in energy systems, which will inform the modelling work of the thesis. The implications of the article findings for this thesis are discussed further in the concluding remarks to this chapter.

Following this introduction, an authorship declaration is provided, followed by the article as published in Sustainable Energy and Fuels (although re-formatted for this thesis). The article includes its own reference list. Following the article, the chapter concluding remarks are provided.

Authorship declaration

This declaration concerns the article entitled: The curious case of the conflicting roles of hydrogen in global energy scenarios	
Publication status **Draft manuscript** ☐ **Submitted** ☐ **In review** ☐ **Accepted** ☐ **Published** ☒	
Publication details	Christopher J. Quarton, Olfa Tlili, Lara Welder, Christine Mansilla, Herib Blanco, Heidi Heinrichs, Jonathan Leaver, Nouri J. Samsatli, Paul Lucchese, Martin Robinius, and Sheila Samsatli. The curious case of the conflicting roles of hydrogen in global energy scenarios. *Sustainable Energy and Fuels*, 4:80-95, 2020.
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Candidate's contribution to the paper	The candidate contributed to / considerably contributed to / predominantly executed the... Formulation of ideas: 10% - The initial ideas were discussed and formulated by all of the co-authors at a workshop. I developed these ideas further for the article. Design of methodology: 50% - Following the workshop, S. Samsatli and I jointly developed the initial arguments into a basic article narrative. Experimental work: 50% - I coordinated the review and analysis work that was carried out. O. Tlili and L. Welder provided the initial literature review, and H. Heinrichs provided the analysis of the effect of emissions reduction targets on scenarios. I reviewed additional material to support and develop these contributions. Presentation of data in journal format: 80% - I developed the initial paper draft, including all figures. All co-authors provided comments on the draft and additional text. S. Samsatli made final edits to the manuscript and helped address the reviewers' comments.
Statement from candidate	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.

Signed		**Date**	16/11/2020

Article:

The curious case of the conflicting roles of hydrogen in global energy scenarios

Abstract

As energy systems transition from fossil-based to low-carbon, they face many challenges, particularly concerning energy security and flexibility. Hydrogen may help to overcome these challenges, with potential as a transport fuel, for heating, energy storage, conversion to electricity, and in industry. Despite these opportunities, hydrogen has historically had a limited role in influential global energy scenarios. Whilst more recent studies are beginning to include hydrogen, the role it plays in different scenarios is extremely inconsistent. In this perspective paper, reasons for this inconsistency are explored, considering the modelling approach behind the scenario, scenario design, and data assumptions. We argue that energy systems are becoming increasingly complex, and it is within these complexities that new technologies such as hydrogen emerge. Developing a global energy scenario that represents these complexities is challenging, and in this paper we provide recommendations to help ensure that emerging technologies such as hydrogen are appropriately represented. These recommendations include: using the right modelling tools, whilst knowing the limits of the model; including the right sectors and technologies; having an appropriate level of ambition; and making realistic data assumptions. Above all, transparency is essential, and global scenarios must do more to make available the modelling methods and data assumptions used.

Abbreviations: CAES: Compressed Air Energy Storage; CC: Carbon Capture; CCS: Carbon Capture and Storage; CCU: Carbon Capture and Utilisation; ER: Energy Revolution; ETP: Energy Technology Perspectives; FCEV: Fuel Cell Electric Vehicle; GEA: Global Energy Assessment; GHG: Greenhouse Gas; H2FC: Hydrogen and Fuel Cell; HDV: Heavy Duty Vehicle; LDV: Light Duty Vehicle; PEM: Proton Exchange Membrane; PHS: Pumped Hydro Storage; SMR: Steam Methane Reforming; UG: Underground; WEC: World Energy Council; WEO: World Energy Outlook.

3.1 Introduction

In order to combat climate change there is increasing interest in achieving net-zero greenhouse gas (GHG) emissions before the end of the century [1]. Energy systems decarbonisation is an essential part of this, as energy sectors contribute around three-quarters of global GHG emissions [2].

Renewable energy technologies have progressed tremendously in recent decades, now offering economically credible alternatives to fossil fuels in many sectors [3]. However, these technologies are fundamentally different to fossil fuels, so a like-for-like replacement is not possible. Renewable resources such as wind and solar are diffuse and intermittent, creating new challenges for matching energy supplies to demands, in both time and space [4, 5]. Furthermore, fossil fuels have unrivalled storage capabilities. It is essential to find low-carbon energy storage options, for temporal balancing of supply and demand, and use in transport [6]. We need to develop technologies that will enable increased energy systems flexibility and interconnectivity, while maintaining reliability and stability [7, 8].

In this context, hydrogen has potential. Apart from small reserves of "natural" hydrogen [9], hydrogen is not a resource that can be extracted at scale in the same way as fossil fuels. However, it can be produced with minimal GHG emissions, for example through electrolysis powered by renewable electricity [10], or from bioenergy or fossil fuels with carbon capture and storage (CCS) [11]. Hydrogen has many possible energy applications, including for heating, transport, industry, and electricity generation [12, 13].

Energy scenarios can provide valuable insights into possible future trajectories of energy systems. Many different national, regional and global energy scenarios exist. Some scenarios, such as those produced by global institutions (e.g. [14, 15, 16]), can be very influential to political discourse.

However, energy scenarios are generated using various methods and, given the complexity of the systems being represented, it is unsurprising that the scenarios produce differing results. In particular, the prominence of hydrogen in different scenarios varies noticeably. Hanley et al. [17] reviewed the role of hydrogen across different energy scenarios, finding a range of results regarding the uptake of hydrogen. Whilst many scenarios include some hydrogen in the transport sector, uptake of hydrogen in other sectors varied significantly depending on the emphasis in the scenario design. Furthermore, the review found a correlation between the level of ambition (e.g. decarbonisation or renewables integration targets) and the contribution of hydrogen in the scenario results.

Given hydrogen's potential to transform energy systems, the variation in its contribution in global energy scenarios is surprising. Whilst Hanley et al. [17] identified some of the trends in hydrogen prevalence, they did not explore the reasons for differing results in detail.

In this perspective, we assess hydrogen's potential as a contributor to energy systems, and examine the methods used in global energy scenarios in order to understand the reasons for differing results regarding hydrogen. We focus on global energy scenarios produced by prominent institutions, as these are typically the most influential. The entire scenario development process is considered, including conceptualisation, model construction, and input data. Based on this analysis, we suggest some best practices for energy scenarios so that they can provide the best insight, and correctly quantify the potential of energy technologies such as hydrogen.

Section 3.2 provides an overview of hydrogen as an energy carrier. Section 3.3 provides details of hydrogen prevalence in scenarios from 12 global studies. In Section 3.4, the reasons for varying results between scenarios are discussed. Finally, some conclusions and suggestions for best practice in scenario development are provided in Section 3.5.

3.2 Opportunities for hydrogen in energy systems

There are many possible pathways for hydrogen in energy systems and in some cases they are already being realised in real projects. In this section, the main pathways are summarised; an overview is provided in Figure 3-1, whilst Pivovar et al. [18] describe them in more detail.

Currently, most hydrogen is produced from fossil fuels, such as reforming of natural gas or gasification of coal. Similar processes can be used to convert biomass feedstocks to hydrogen [19]. Water electrolysis has been used to produce hydrogen in certain industrial applications for over a century, but in recent decades it has seen growing interest due to newly emerging technologies and availability of low-cost electricity [10]. Many future projections for hydrogen are based on large contributions from electrolysis but there are other new technologies emerging, such as thermolysis and photolysis, that may offer a more efficient use of thermal or solar energy for hydrogen production [20].

Applications of hydrogen include conversion to electricity using a fuel cell [19], contributing to industrial processes [21, 22], and combustion for heat and/or power generation

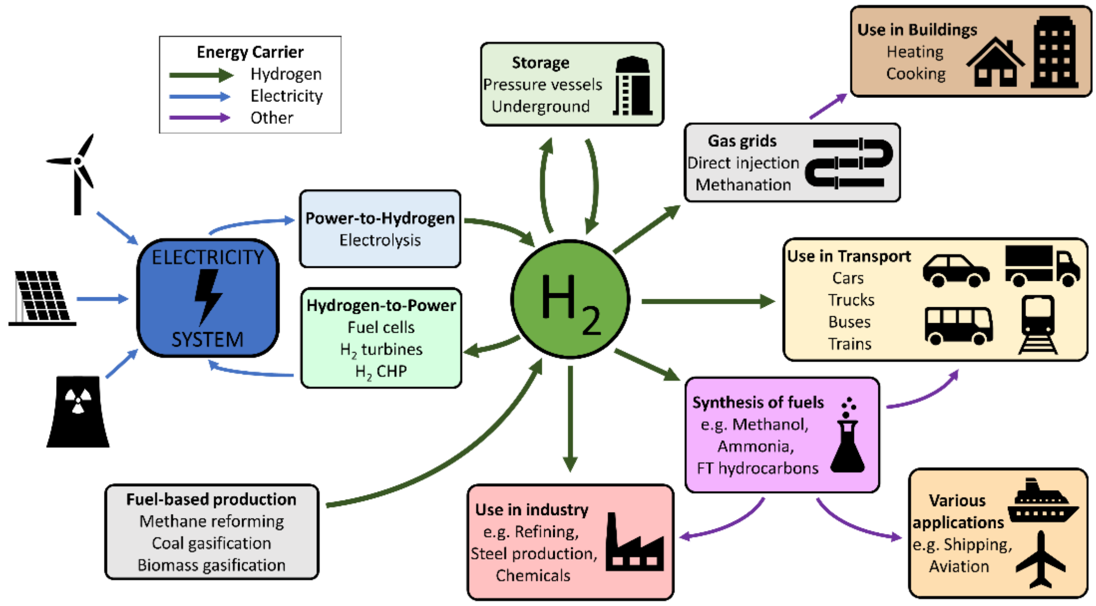

Figure 3-1: **Overview of key hydrogen production and usage pathways.** With multiple production options and applications, hydrogen could be valuable in providing flexibility and sector-coupling to energy systems.

[23]. Hydrogen can be stored in quantities from MWh to TWh, for example in pressurised cylinders or underground in salt caverns, depleted oil and gas reservoirs and saline aquifers [19, 24]. Pressurised hydrogen storage has a volumetric energy density greater than 500 kWh/m^3, far exceeding low-carbon energy storage alternatives (up to 1.5 kWh/m^3 for pumped hydro storage (PHS) and 12 kWh/m^3 for compressed air energy storage (CAES)) [5].

Hydrogen's high energy density makes it particularly interesting for system-wide energy balancing. Hydrogen could be manufactured from electricity at times of excess supply, stored, and later converted back to electricity or used for other purposes at times of high demand [10]. However, hydrogen storage round-trip efficiencies are around 20-36%, which is low compared to alternatives (PHS: 70-85%; CAES: 65-80%; battery: 86-95%) [6]. Therefore, the value of hydrogen energy storage depends on the trade-off between the benefits of time-shifting bulk energy, and the costs of the efficiency losses.

Whilst hydrogen for electricity storage has not yet been deployed at large scale, already several projects have deployed electrolysers to absorb electricity from wind farms, to be stored and used at a later date in various applications (for example Energiepark Mainz [25] and Lam Takhong [26]). For the 2020 Olympics, Tokyo plans to power the Olympic village with hydrogen from solar-powered electrolysis [27].

Hydrogen's suitability for storage also makes it appealing as a transport fuel. A hydrogen fuel tank and fuel cell can provide the electricity supply for an electric vehicle, or hydrogen can be burned in an internal combustion engine. Hydrogen is seen as a possible low-carbon fuel in transport sectors that require long ranges, such as road freight, rail and shipping [13, 28]. Hydrogen in passenger vehicles could also offer greater driving ranges, faster refuelling times and in some cases lower cost of ownership compared to battery electric vehicles [29, 30].

The transport sector has seen the greatest interest in hydrogen so far and there is considerable interest globally in expanding the use of hydrogen as a transport fuel. There are over 350 hydrogen fuelling stations worldwide, across the Americas, Europe, Asia and Oceania [31]. Hydrogen buses are in use in many cities around the world including in USA, Japan, China and several countries in Europe [32, 33]. Alstom have developed a hydrogen train, the first of which went into operation in Lower Saxony, Germany in 2018 [34].

Hydrogen is already a key chemical component in many industrial markets: the main applications include ammonia synthesis (55% of hydrogen demand); hydrocracking and hydrodesulphurisation in refineries (25%); and methanol production (10%) [35].

Nonetheless, the "hydrogen economy" is still in the early stages of development. In most applications, there has been limited deployment of hydrogen beyond demonstration projects [36]. Most of the hydrogen used today is produced on-site for specific applications. Consequently, there has been limited infrastructure development other than for transportation between chemical manufacturing sites. Today, there are around 16,000 km of hydrogen pipelines globally [12] compared to 2.91 million km for natural gas [37]. For expansion beyond the chemical sector, it will be necessary either to build new hydrogen infrastructure, or to utilise existing infrastructure (e.g. partial injection or conversion of existing gas networks) [36].

Low-cost, low-carbon hydrogen production at scale is also still a challenge. Conventional production such as steam methane reforming (SMR) would require carbon capture and storage (CCS) to minimise GHG emissions, but this adds around 45% to the cost [11], and CCS deployment remains limited. Low-carbon production of hydrogen using electrolysis requires both significant electrolysis capacity and sufficient low-carbon electricity production. Although costs of renewable electricity are falling rapidly with increasing installed capacity [3], electrolysis installed capacity is low and reductions in capital costs through economies of scale are still required [38, 39]. Lastly, fuel cell costs are relatively high (around $280 /kW [40]), and manufacturing scale up is required to make hydrogen competitive with other energy carriers.

Hydrogen can also be combined with captured CO_2 in carbon capture and utilisation (CCU) processes. CCU can produce useful energy carriers that are already in use and have existing infrastructures, such as methane, methanol and liquid hydrocarbons [41]. The CO_2 used in CCU could be captured from fossil sources, but increased environmental benefit would be achieved if the CO_2 were captured from biomass or directly from the air [42]. The challenges for CCU are energy losses associated with the additional conversion step (20-35% [43]), and high costs compared to the fossil alternatives they would replace (e.g. CCU transport fuel may cost €30 /GJ, compared to €15 /GJ for petroleum-based fuels [44]). Hydrogen can also be combined with nitrogen to produce ammonia, which has advantages for storage and transport, and can be used for heat and power generation [45].

3.3 Global energy scenarios and the representation of hydrogen

3.3.1 Energy scenarios

Energy scenarios can address the uncertainties surrounding the socio-technical evolution of energy sectors. Scenarios can be qualitative, relying on inputs from experts and stakeholders, or quantitative, usually based on energy systems models [46]. Scenario development aims to construct possible futures and the paths leading to them, and can guide strategic decision-making processes, for example for maintaining long-term energy supply-demand balances and optimising investment decisions. Consequently, these scenarios can be highly influential to the future of the technological "ecosystem" in different sectors. Due to the size and complexity of the energy systems being represented by energy scenarios, simplifying assumptions must be made, and these can have significant implications for the scenario results.

Several reviews of model-based scenarios and the modelling tools they use have been carried out, highlighting a variety of methods and results. Pfenninger et al. [47] reviewed energy systems models in the context of present-day energy systems, and identified several challenges that these models face, stemming from the increased complexity of modern energy systems. The review also provided recommendations for modelling practice, encouraging innovation with modelling methods, appropriate handling of uncertainty and modelling transparency. Meanwhile, Gambhir et al. reviewed energy scenario results, finding that the level of climate change ambition has a significant effect on the scenario results [48]. Lopion et al. [49] investigated trends in energy system models developed for national greenhouse gas reduction strategies, in the context of underlying research questions and their shift over time, and found that there is an increasing need for high temporal and spatial resolutions.

As Hanley et al. [17] found, the prominence of hydrogen varies significantly between energy scenarios. Whilst many of the scenarios Hanley et al. studied included some hydrogen in the transport sector, hydrogen prevalence in other sectors was low, except where hydrogen was a specific focus of the study. The scenarios that focus on hydrogen, such as the IEA Energy Technology Perspectives (ETP) 2°C "high hydrogen" scenario, have begun a trend of greater hydrogen representation, and hydrogen prominence is growing in the most recent scenarios.

In this perspective, we discuss why there has been an historical absence of hydrogen in global energy scenarios, and why that is beginning to change. Many energy scenarios exist at regional and national levels, such as the EU Reference scenario [50], ASEAN Energy Outlook (SE Asia) [51], IDB Lights On scenario (Latin America) [52], EIA Annual Energy Outlook (USA) [53], China Renewable Energy Outlook [54], the Japan Strategic Energy Plan [55], and the Deep Decarbonization Pathways Project (various countries) [56]. However, in this perspective we focus on global scenarios with the greatest international impact.

The 12 studies that were considered are shown in Table 3.1. We focus on the scenarios from 10 model-based studies and also consider two hydrogen-focussed qualitative scenarios: the IEA Hydrogen and Fuel Cells Technology Roadmap [29] and the Hydrogen Council "Scaling Up" scenario [57], as they provide a counterpoint for the potential for hydrogen, as perceived by experts and stakeholders.

3.3.2 Hydrogen representation in global energy scenarios

Between the 35 scenarios considered there is significant variation regarding which hydrogen technologies and end-use applications are considered, and the level of detail with which they are included. In Figure 3-2, the level of representation of these hydrogen technologies is presented, including whether the technology is modelled, whether data assumptions are provided, and whether hydrogen contributes to the final results. Whilst there are conflicts in the prominence of hydrogen between scenarios, what is common is that limited specific techno-economic information is provided. Often, concepts are discussed but with little detail, so it is difficult to understand how these concepts are represented and what assumptions have been made.

Table 3.1: Details of the studies and scenarios that were reviewed. Global studies from influential institutions were chosen, focussing on quantitative (model-based) scenarios. Two qualitative scenarios were also included.

Study	Abbreviation	Model used	Scenario end year	Scenarios
World Energy Outlook (IEA) 2016 [58]	WEO 2016	World Energy Model + MoMo	2040	Current Policies New Policies 450 Scenario
World Energy Outlook (IEA) 2017 [59]	WEO 2017	World Energy Model + MoMo	2040	Current Policies New Policies Sustainable Development
World Energy Outlook (IEA) 2018 [14]	WEO 2018	World Energy Model + MoMo	2040	Current Policies New Policies Sustainable Development The Future is Electric
The Grand Transition (WEC) 2016 [15]	WEC	GMM	2060	Hard Rock Unfinished Symphony Modern Jazz
REmap (IRENA) [60]	REmap	E3ME	2050	Reference REmap
Energy Technology Perspectives (IEA) 2016 [61]	ETP 2016	ETP TIMES + MoMo	2050	6DS 4DS 2DS
Energy Technology Perspectives (IEA) 2017 [62]	ETP 2017	ETP TIMES + MoMo	2060	RTS 2DS B2DS
Energy Revolution (Greenpeace) [63]	ER	REMix	2050	Reference E[R] ADV E[R]
Shell scenarios (Shell, 2018) [16, 64]	Shell	Shell World Energy Model	2100	Mountains Oceans Sky
Global Energy Assessment (IIASA) [65]	GEA	MESSAGE + IMAGE	2050	Supply (Conv. Trans) Mix (Conv. Trans) Efficiency (Conv. Trans) Supply (Adv. Trans) Mix (Adv. Trans) Efficiency (Adv. Trans)
Hydrogen Council (2017) [57]	H2 Council	Qualitative	2050	Hydrogen - scaling up
Technology Roadmap: Hydrogen and Fuel Cells (IEA) [29]	H2FC Roadmap	Qualitative	2050	2DS High H2

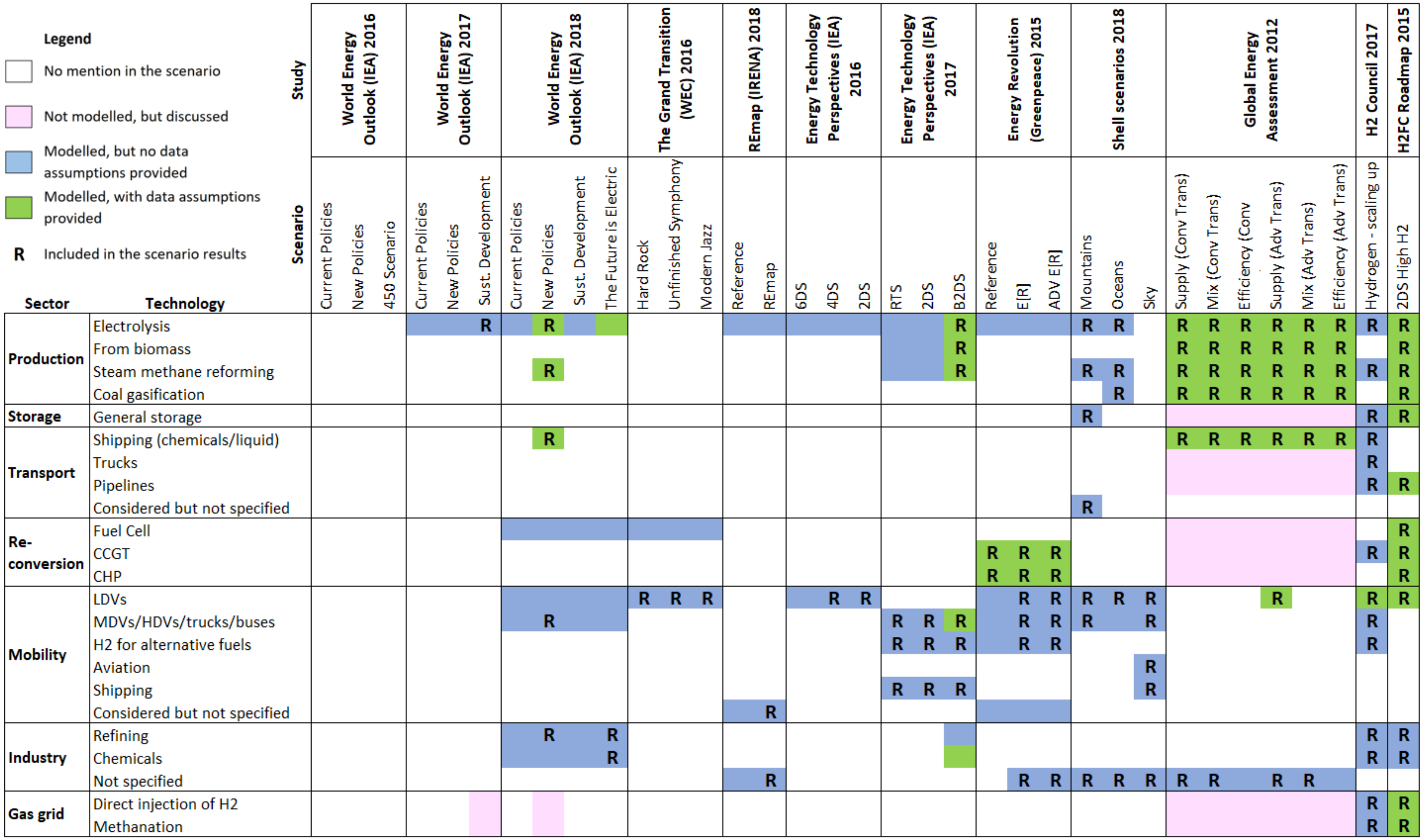

Figure 3-2: **Differing representation of hydrogen in scenarios from 12 global studies.** Hydrogen representation is separated into seven sectors, covering the supply-side (production, storage, transportation), and applications of hydrogen (conversion to electricity, mobility, industry, gas grid). Colours refer to the level of representation in the scenario design; "R" denotes technologies that are included in the results of the scenario. See the legend for more details.

Regarding technologies, hydrogen production is covered in the most detail, and in this case techno-economic assumptions are often provided. Electrolysis is commonly considered, although the technology type is rarely specified (WEO 2018 [14], Shell [16, 64], GEA [65], ER [63], REmap [66]). ETP 2017 specifically considers the more commercially developed alkaline electrolysis, whereas the H2 Council focus on PEM electrolysis, which many expect to overtake alkaline as the favoured technology [39]. The qualitative H2FC road map [29] is the only study to consider solid-oxide electrolysis.

Several studies discuss other production options, such as SMR, coal gasification and biomass-based production. These production options are typically mentioned when comparing hydrogen production costs (WEO 2018 [14], H2FC Roadmap [29]) or as a transitional step to fully decarbonised hydrogen (Shell [16, 64]). The techno-economic assumptions related to these technologies (mainly SMR/SMR+CCS) are often presented, and it is observed that the costs of electrolysis and SMR+CCS are converging [29].

Other hydrogen infrastructures, such as transportation and storage, receive little coverage in most studies. A few studies discuss storage, but provide no data, suggesting it is not modelled (GEA [65], ER [63], H2 council [57]). Hydrogen transportation receives slightly more coverage, most commonly shipping for global transportation (WEO 2018 [14], H2 Council [57], GEA [65]). In general, limited data is provided for transportation, so it is unclear what assumptions are made (e.g. how transportation is costed), or whether it is considered at all.

End-use applications are described in more detail in the scenarios. The most prominent end-use is mobility, which is considered in some form in all but WEO 2016 [58] and WEO 2017 ([59]. Fuel Cell Electric Vehicles (FCEVs) for light-duty passenger vehicles (LDVs) are predominant but heavier duty vehicles (HDVs, e.g. trucks and buses) are also discussed in more-recent studies (though rarely quantified). Instead, discussion is more focussed on societal issues, such as government policies. The qualitative studies [29, 57] provide more techno-economic data for HDVs. Finally, there is some interest in hydrogen for alternative fuels but limited details on techno-economic assumptions are provided (ER [63], ETP 2017 [62], H2 Council [57]).

Beyond mobility, other applications for hydrogen are discussed in less detail. Several studies consider industrial applications, with refining applications such as steel and iron, and chemical applications such as ammonia production being the most popular. Electrification of processes via electrolysis is mentioned (WEO 2018 [14]), but again with little detail. Interactions with the gas grid (either direct hydrogen injection or methanation) are often mentioned in discussion, but rarely quantified in the results

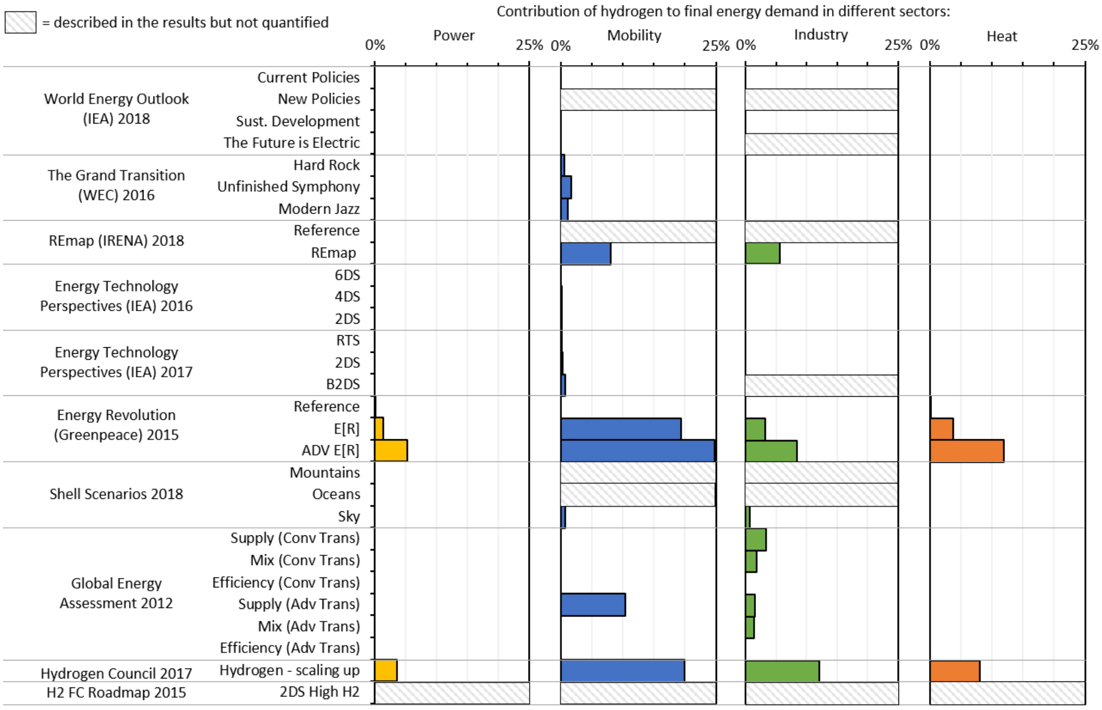

Figure 3-3: **Contribution of hydrogen to final energy demand in 2050 in power, mobility, industrial and heat sectors for a range of scenarios.** Where studies state the inclusion of hydrogen in the results without precisely quantifying it, values have either been estimated by the author (IEA ETP 2016, Shell Sky and H2 Council scenarios), or the result has been denoted by a hashed box.

(GEA [65]; WEO 2017 [59], H2FC Roadmap [29], H2 Council [57]). Finally, conversion of hydrogen to electricity and heat is rarely mentioned. Where it is considered, the most common technologies are fuel cells, gas turbines and combined heat and power applications. The ER scenarios [63] are the only ones to include these applications in the scenario results.

3.3.3 Conflicting roles of hydrogen in global scenario results

The variability in representation of hydrogen in scenarios leads to conflicts in the level of contribution of hydrogen in the scenario results. Figure 3-3 shows the contribution of hydrogen to final energy demand in 2050 in different sectors, for each of the scenarios that includes hydrogen in its results.

Overall, the scenarios indicate that hydrogen has the most potential in the mobility sector. Most scenarios have some level of hydrogen in this sector but they offer conflicting levels of contribution: in many cases this is less than 2% of transport energy demand in 2050 (e.g. WEC [15] and ETP 2017 [62] scenarios); whereas the Greenpeace ER and Adv ER scenarios give contributions as high as 19% and 25%, respectively [63].

Similarly, the contribution of hydrogen in the industrial sector ranges between 0.7% of 2050 industrial demands (Shell Sky [16]) and 12% (H2 Council [57]) but many scenarios do not include it at all.

The focus between these two sectors can also shift between scenarios: the Grand Transition scenarios suggest hydrogen should contribute to the mobility sector and not to industry whereas several of the Global Energy Assessment scenarios advocate the opposite.

The Greenpeace scenarios [63] are the only quantitiative scenarios to include hydrogen in the results for the power and heating sectors and both qualitative scenarios also include it (H2FC roadmap [29] and H2 council [57]).

3.4 Discussion: what must scenarios do to represent hydrogen fairly?

From the results in Section 3.3, and from previous reviews, there is clearly significant variation between scenarios concerning the prominence of hydrogen in energy systems. Although most of these scenarios rely on energy system models, the representation in these models is not sufficient to capture all of the advantages of hydrogen. In this section, we examine the key steps in quantitative scenario development, to understand why differing results may arise, and consider what scenario developers should be doing to make sure hydrogen, and other flexibility options (such as alternative storage technologies, demand-side response, electricity grid expansion and interconnectivity [67]), are appropriately represented.

3.4.1 Scenarios must use appropriate modelling tools

Energy systems models form the basis of most quantitative energy scenarios. A vast number of energy system modelling tools exist and can be categorised in different ways, including simulation vs optimisation, top-down vs bottom-up, etc. In a review of computing tools for energy systems, Connolly et al. [68] identified 68 different energy system modelling tools. Lopion et al. [49] reviewed 24 energy system models in detail, also categorising them as above, and found a clear trend towards techno-economic bottom-up optimisation models in order to answer current research questions.

Each energy systems model is designed for its own unique purpose and has its own strengths and weaknesses. Some of the oldest models were developed in the second half of the 20th century to help understand energy systems in the context of the oil crisis and concerns over security of energy supply [47]. These models are the predecessors of many models in use today, where due to climate change, we face significantly different energy challenges. It is important that energy systems models in use today are appropriately designed to represent the challenges we face in the twenty-first century.

The most difficult task for modern day energy systems models is to capture the full degree of variability and complexity that exists in energy systems. Traditionally, energy systems were centralised and underpinned by fossil fuels. In the electricity sector for example, supply would be made up of either base-load or dispatchable generation. However, as more and more renewable sources such as solar and wind are introduced to aid decarbonisation, systems are becoming more spatially distributed, technologically diverse and temporally variable. Meanwhile, new technologies and increased interconnectivity are enabling more interaction between different energy sectors, known as "sector-coupling" [69]. To ensure that energy system models not only provide an accurate representation of energy systems but also do not miss the potential of new technologies such as hydrogen-based technologies, they must capture the required level of temporal, spatial, technological, and inter-sectoral detail.

3.4.1.1 Models must capture sufficient temporal detail

Many large-scale energy models are unable to represent the time scales at which flexibility technologies such as electrolysers, hydrogen storage and fuel cells are most useful. For example, traditional energy system models typically use representative time slices, such as day, night, and peak for a series of day types throughout the year. In some cases, within-day chronology is retained, meaning that it may be possible to model some level of intraday storage. However longer-term chronology is rarely retained, thus losing the ability to represent long-term storage [70, 71], which is an area where hydrogen is seen to have strong potential [6, 72]. Novel methods for modelling seasonal storage are beginning to emerge [73, 74] but they have not been applied to any of the global energy scenarios. Meanwhile, short-term dynamics, such as electricity dispatch on a sub-hour basis, are also not modelled by large-scale energy models. This means that another opportunity for hydrogen, as a short-term load balancer through electrolysis [75, 76], is also missed. The effects of under-representing temporal detail in energy scenarios have been explored and it has been found that investment optimisations will underestimate the contribution of dispatchable power generation and instead favour baseload and intermittent renewables [77]. It is therefore likely that flexibility options such as those based on hydrogen are also being under-valued.

The challenge for large-scale energy systems models is to capture the full range of time scales necessary. The models are designed for long-term investment planning, and therefore require multi-decadal time horizons. However, the dynamics of the energy system at all time scales (including seasonal, weekly, daily, and sub-hourly) are important to how the system should be designed and operated. Approaches to improve the accuracy of the time-slicing method include using a higher resolution of time intervals; probabilistic representation of the loads and renewable energy supplies; and using real historical data for the time intervals [70]. However, each of these approaches suffers the same issue of failing to maintain chronology across the whole time horizon, hence some representation of flexibility is lost. Alternatively, energy systems models can be soft-coupled to power sector models, taking advantage of the latter's improved temporal representation [70]. However, this approach can increase overall complexity, as there are two separate models to maintain and run. Furthermore, due to the required iteration between the two models, there is no guarantee that an optimal solution will be obtained.

3.4.1.2 Models must capture sufficient spatial detail

As well as temporal flexibility, hydrogen can provide spatial flexibility to energy systems. Hydrogen transportation by road, pipeline and shipping provide opportunities for the transportation of energy that cannot be provided by other energy carriers (e.g. electricity). Large-scale (e.g. global) energy models usually have limited spatial detail, using average resource demands and supplies over large spatial regions [47]. Consequently, they do not capture the value of energy transportation at a smaller scale, such as across country. Furthermore, spatial variabilities in solar and wind generation will affect supply profiles across a region: this "spatial smoothing" cannot be fully represented with too coarse a spatial resolution [70].

One option for improving this modelling would be to include a higher spatial resolution but this would significantly increase the complexity of the model. Alternatively, models should seek to use representative data and relationships to value within-region energy transportation and distribution.

3.4.1.3 Models must appropriately represent technologies and inter-sectoral connectivity

Technological representation in large-scale energy models is often restricted to blanket details for each technology type, rather than representing individual technologies or plants [77]. Consequently, realistic operation of plants, taking their flexibility constraints into account, is not modelled. This is not helped by the lack of temporal resolution and chronology.

To improve technological representation, approaches include further modelling of ancillary markets (e.g. flexibility markets), and broader constraints that attempt to represent the overall behaviour of many individual technologies of a given type [70].

Finally, hydrogen is central to several sector-coupling options, including power-to-gas (for the gas grid) [36], power-to-heat [78], power-to-liquids [79], and power-to-ammonia [80]. Energy systems models need to include the opportunity for transfers of energy between sectors, as this can unlock potential for cost and resource efficiency savings.

3.4.1.4 Models must represent the complexity of consumer behaviour

Uptake of new technologies is not only driven by cost or efficiency-based metrics for the entire energy system, but also by consumer choice, dependent on social factors and personal preference. For example, market adoption of FCEVs is sensitive to consumer perception of factors such as driving range, battery life, depreciation and capital cost. Furthermore, vehicle uptake is affected by consumer perception in the used vehicle market.

There are significant variations between models regarding how consumer choices are represented, for example the inclusion and relative importance of different utility factors representing consumer choice. Improvements in modelling can be achieved with more readily available data on elasticities and utility factors. Furthermore, more a detailed representation of different technology types (e.g. different weight and range categories for vehicles) will allow for a more accurate representation of consumer choice.

3.4.1.5 Models must remain manageable and user-friendly

Increasing computational power means that larger, more complex and more realistic models can be developed. However, this greater detail can introduce difficulty for the model users, in terms of managing the much larger datasets that are required as inputs and generated as outputs, analysing the results and communicating them to a general audience, such as policy makers and the general public. The challenge for energy systems models is therefore to use appropriate techniques such as those described above whilst preventing the model from becoming too difficult to use and to communicate. Although the detailed outputs of a complex model can be summarised using averages and high-level metrics, some of the important insights can only be understood from the details and presenting these in a manner that is easy to understand remains a key goal and challenge.

3.4.1.6 Model methodologies must be transparent

Due to the complexities in representing the details of energy systems, it is important that when scenarios are presented, the methodologies behind them are shared. The fact that these models are being used to predict what future energy systems may be, often many decades into the future, means that there is no real-life system against which the models can be validated. As most energy system models use optimisation and today's energy systems are far from optimal, it is difficult even to validate these models against current data. For this reason, it is important that the mathematical formulations behind the models be published so that they can be appropriately peer reviewed. However, this practice is very rare among the global energy scenarios: none of the scenarios reviewed in Section 3.3 have published the mathematical formulations of their models. Indeed, most give no or very little information regarding the modelling approaches used and only the IEA ETP studies [61, 62] describe qualitatively the modelling framework that is used to generate the results (four soft-linked models are used, including ETP TIMES models for energy conversion and industry, the MoMo model for transport, and the Global buildings sector model for buildings). One might argue that if the results over a wide range of scenarios appear sensible, behave as expected and can be explained, then that is a sufficient test. However, since many modelling assumptions must be made even in complex models, different formulations of the same physical phenomena are possible and these can result in different but still sensible results.

One barrier to the publication of a model's mathematical formulation is the intellectual property rights of the organisation that developed the model. This is understandable, but the IP is more than just the mathematical constraints employed by the model. It is not practical to publish all of the know-how in the implementation and solution of the model (the minute details required to obtain robust and reliable solutions) and there are many other elements to the IP: data management, user interface, results management and analysis.

The main advantage of model transparency is that this allows other modellers to review the model, highlight any deficiencies and suggest improvements. This will provide researchers and policy makers with the confidence that the results of the scenarios are truly meaningful and that they can be taken forward with real enthusiasm. This can only really be possible by publishing the mathematical formulation of the model, as has been done in other similar areas (see e.g. [72, 81, 82, 83, 84, 85]).

Finally, given that models each have their own strengths and weaknesses, transparency enables scenario developers to choose the model that is best suited to the application. Where energy scenarios are used to inform policy decisions, decision making cannot be considered fully transparent if the methodologies behind the modelling are not themselves transparent.

3.4.1.7 Challenges and pitfalls

We have argued that models must be much more detailed, and therefore complex, than are currently being used in global energy scenarios. Including features such as high spatial and temporal resolutions, uncertainty analysis, consumer behaviour and including a large range of technologies and energy carriers in a model is extremely challenging. Of course, the models should be made only as complex as is necessary to represent all of the features and details of hydrogen (and other) technologies that may play a role in the future energy system (such as rapid-response load balancing technologies). Modellers and scenario planners should follow a structured approach to developing new models similar to the one below:

1. Describe the purpose of the study carefully
2. Define the scope so that the purpose can be achieved satisfactorily and with sufficient accuracy
3. Build the simplest model that can accurately represent all of the features and interactions of the system defined in the scope
4. Provide assumptions and limitations
5. Discuss results in light of assumptions and limitations, acknowledging that the model is imperfect

Deciding the necessary level of detail and accuracy is itself a difficult decision but this can be helped by performing smaller studies involving particular technologies to determine what level of spatial and temporal detail are required. The greatest difficulty for a modeller is when the required level of detail is so high that the model becomes computationally very demanding but further simplifications make the model no longer fit for purpose.

It is understandable that time pressure in intractability tempt researchers into oversimplifying models in order to obtain results. This is a pitfall that needs to be avoided or at least taken with extreme caution. The results and conclusions obtained from an oversimplified model can be misleading and possibly erroneous. In the context of hydrogen, if a technology does not appear in the results then it is not possible to determine whether this is because of an inherent disadvantage of the technology or whether it is due to the inadequacy of the model to represent the technology's benefits.

Despite the challenges of including an unprecedented level of detail in energy system models, these are not insurmountable goals. As has been mentioned, techniques have already been developed that allow national energy systems to be optimised with high levels of spatial and temporal disaggregation. With increasing computing power and further research in to advanced techniques and algorithms, more complex and detailed models will be possible in the near future. Scenario developers should be aiming to take advantage of these developments in order to obtain more reliable, and perhaps surprising, results.

3.4.2 Scenarios must be designed appropriately

Scenario design, including which sectors and technologies are included, what the level of ambition is, and what performance metrics are used, has a significant influence on scenario results. Scenario design will partly be determined by the capabilities of the model used. However, many decisions will also be made by the developer.

3.4.2.1 Scenarios must include all relevant sectors

As the results in Section 3.3 show, there is significant variation in the sectors that are included in different scenarios. Some sectors, such as mobility, are represented in almost all scenarios, but others have significant variability. For example, hydrogen is widely discussed as a key decarbonisation option for industry, as shown by its strong representation in the qualitative scenarios. Furthermore, in almost all quantitative scenarios where hydrogen in industry is included as an option, it contributes to the final results (e.g. ReMap, Shell and the Global Energy Assessment). However, several studies omit hydrogen in industry altogether, such as the early WEO and ETP scenarios, the WEC Grand Transition, and even the ambitious Energy Revolution scenarios. Given that hydrogen does appear in the results of many of the scenarios that included it, it is reasonable to wonder if it would have also played a role in the other scenarios had they included it.

The other applications of hydrogen (re-conversion, gas grid) show similar variability between different scenarios and there is no consistent trend regarding which scenarios include which sectors. For studies that have re-produced scenarios in consecutive years (WEO, ETP), it is noticeable that the newer scenarios have a more comprehensive inclusion of sectors than the older scenarios. For example, WEO 2018 had at least some discussion of re-conversion, mobility, industry and the gas grid, whereas the previous iterations of the study (2016 and 2017) did not consider any of these sectors. Assuming that the modelling methods for these scenarios are not changed significantly from one year to the next, this again suggests that had these sectors been included earlier, they would have been seen in the scenario results. This shows the importance of including the sectors that have the most potential and suggests that awareness of the potential solutions of applications such as hydrogen is important for their prevalence in scenario results.

3.4.2.2 Scenarios must be technology rich: a technology not included will not appear in the results

As well as the importance of which sectors are included in a given scenario, it is important to consider which specific technologies are included. Again, Figure 3-2 shows the variability in the hydrogen technologies that are included in each scenario. Figure 3-2 would suggest that electrolysis is a key technology for hydrogen, as it is included in almost all scenarios. However, some scenarios even omit this technology. Despite referring to hydrogen as a transport fuel and the use of fuel cells, the WEC Grand Transition [15] makes no reference to electrolysis or any other hydrogen production technology. The scenarios with a richer representation of hydrogen production technologies (e.g. fossil or biomass-based options as well as electrolysis) typically also include a greater representation of hydrogen in the scenario results.

A challenge for energy scenarios is to keep pace with and to estimate future technology developments so that they can be appropriately represented in scenarios for energy systems several decades in the future. For example, solid oxide electrolysis is a technology with significant interest due to its potential for higher efficiencies, reversible operation and co-electrolysis with carbon dioxide [38]. This is reflected in the technology's inclusion in the H2FC Roadmap [29]. However, the technology currently has a low level of commercial development, so is not included in any other scenarios.

Some of the most widely discussed advantages of hydrogen are its usefulness as an alternative energy vector, particularly for large-scale storage and transportation. However, these technologies are omitted from many scenarios. Hydrogen has a high volumetric energy compared to alternative energy storage options, so it is seen to have potential for large scale energy storage applications, for example for balancing electricity supplies and demands in systems with large penetrations of intermittent renewable energy. This potential is reflected in the qualitative scenarios, as well as the Shell and GEA scenarios, however no other scenarios include hydrogen storage.

Similarly, another advantage of hydrogen is that it can be transported easily at a range of scales. Unlike electricity, hydrogen can be shipped across long distances internationally, creating the potential for global supply chains [86]. Pipelines also provide the opportunity for hydrogen transportation, and there is interest in both purpose-built hydrogen pipelines and re-purposing existing natural gas grids [36]. At a smaller scale, hydrogen can also be transported on road by truck. Like storage, hydrogen transportation is hardly included in any of the scenarios.

The omission of these key hydrogen infrastructures is significant, as they are central to what makes hydrogen a potentially valuable energy carrier in future systems. Whilst the technologies for hydrogen production and consumption may not be the most efficient or the lowest cost, benefits arise from the efficiency with which hydrogen can be stored and transported, and hence these infrastructures should be included in energy scenarios.

3.4.2.3 Scenarios must have an appropriate level of ambition

In addition to the technologies and sectors included in the scenario, the level of scenario ambition also influences the prevalence of hydrogen in the results. Most scenarios investigate how an energy system may evolve over time, under existing or expected policies, and can be described as "explorative"; whereas other scenarios impose strict targets on the final energy system and can be referred to as "normative". Reduction of greenhouse gas emissions is a typical target in normative scenarios. While some explorative global energy scenarios can even show an increase in global greenhouse gas (GHG) emissions, normative scenarios often target drastic cuts in GHG emissions, including nearly net-zero emission scenarios.

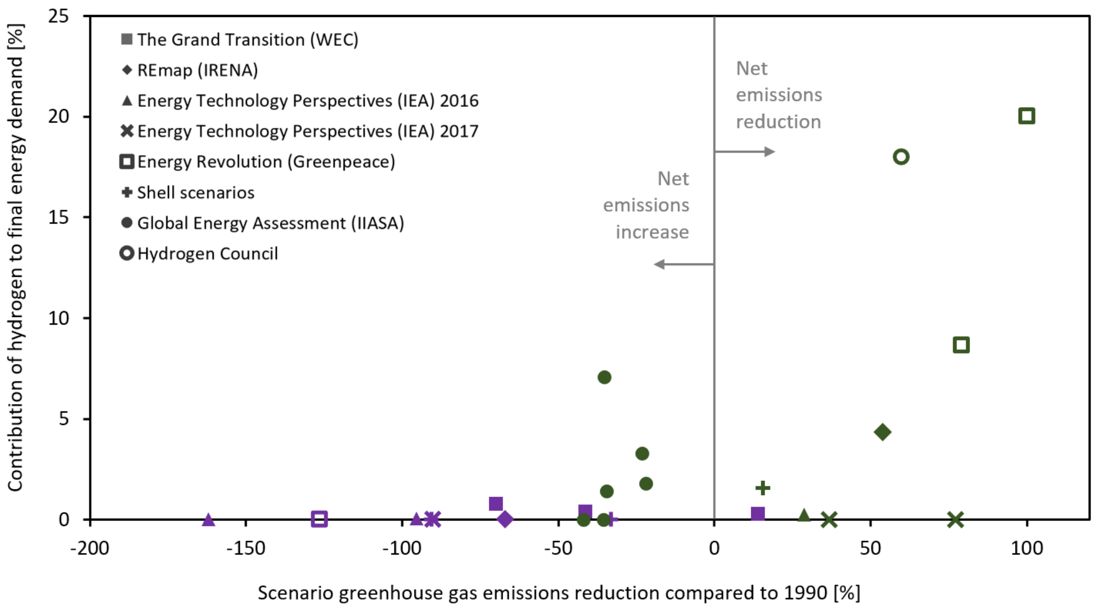

Figure 3-4: **Effect of greenhouse gas (GHG) emissions reduction on hydrogen prevalence in energy scenarios.** A negative GHG emissions reduction represents an increase in emissions over the scenario time horizon. Explorative scenarios are displayed in purple, while normative are displayed in green.

Scenarios with higher levels of GHG reduction ambition show a tendency towards a greater prevalence of hydrogen in their results. Drawing quantitative correlations between GHG reductions and hydrogen prevalence is challenging, due to the tendency for scenarios to discuss hydrogen usage without providing specific data. However, Figure 3-4 shows estimated hydrogen usage as percentage of total final energy demand in several scenarios, compared with the GHG emissions reduction in the scenario. A negative GHG emissions reduction represents an increase in emissions over the scenario time horizon.

Ambitious GHG reduction targets are achieved to some extent with increased uptake of intermittent renewables such as wind and solar. Consequently, energy system flexibility is required to balance electricity supplies and demands. With intermediate decarbonisation objectives, such as an 80% reduction in emissions, this "backup" can be provided by fossil fuels. However, in close to "net-zero" scenarios, nearly any usage of fossil fuels must be balanced by carbon sequestration. Where carbon sequestration is unattractive (due to technical, economic or social factors), alternatives such as hydrogen for energy storage become much more attractive.

Furthermore, with more variable renewable electricity generators on the grid in ambitious GHG scenarios, there is increased complexity in energy markets, for example with increased occurrence of near-zero power prices arising from excess electricity generation. In these situations, there is greater potential for alternative technologies such as power-to-gas to find viable business cases [87, 88].

Finally, scenarios with less ambitious decarbonisation objectives do not always consider the decarbonisation of the more challenging sectors, such as industry or long-haul transport. Certain hydrogen pathways, such as power-to-fuels, are particularly attractive in these sectors [89].

3.4.2.4 Scenarios must consider other objectives

Besides the level of decarbonisation and renewables integration ambition, many other objectives and constraints, such as political interest, social acceptance and national strategies, may be included in a scenario that will affect its outcomes. For example, nuclear power is a politically controversial technology that many countries are choosing to phase out [90]. Other potentially controversial technologies include CCS, and even onshore wind power. Meanwhile there are also resource-based constraints: e.g. some regions have limited biomass potential, limiting this option for future energy systems aiming for energy independence. These choices shape the scenario design and the evolution of the energy system. As these become more constrained, it is possible that hydrogen pathways will emerge as one of the remaining degrees of freedom to achieve ambitious climate targets.

3.4.3 Scenarios must use consistent and substantiated data assumptions

As well as broad scenario design, the thousands of data parameters that are input into each scenario will influence the scenario results.

Typical input data for technologies in energy systems models will include cost data (e.g. capital and operating costs) and performance data (e.g. operating rates, efficiencies, environmental impacts, etc.). For any technology there will be an uncertainty range in these data, depending on how, when and where the technology is installed and operated. As an example, some cost estimates for key hydrogen technologies are shown in Table 3.2, showing the wide uncertainty range in the literature. Energy scenarios are not able to capture this range in every detail, due to the large number of variables already being considered, and consequently must carry out some “averaging”.

Table 3.2: Cost estimates for key hydrogen technologies for present day and 2050

Technology	Unit	Capex		Ref.
		Today	2050	
Electrolyser (Alkaline)	€/kW	800 - 1700	400 - 1200	[38, 91]
Electrolyser (PEM)	€/kW	1300 - 3200	300 - 1600	[38, 91]
SMR (with CC)	€/kW	600 - 1300	400 - 600	[11, 29, 92, 93]
H2 storage (vehicle on-board)	€/kWh	13 - 20	8 (target)	[94]
Fuel cell (vehicle on-board)	€/kW	38 - 152	34 (target)	[94]
H2 storage (UG compressed)	€/kWh	0.1 - 2.0	0.1 – 2.0	[92, 93, 95]
Fuel cell (stationary)	€/kW	640 - 2900	330 - 600	[29]

Energy scenarios also need to capture the changes in cost and performance data that will occur over time. Rapid progress in energy technologies has been seen before, for example in solar PV [3] and lithium-ion batteries [96]. This sort of progress is dependent on the scale of production. Learning curves can be used to estimate improvements in cost and technical performance with increased production rates but estimating the rates of uptake of technologies is challenging, particularly as these can be influenced by government policy.

Large-scale energy scenarios are typically based on policies that are already in place and free-market decisions. For the future, usually broad policies (e.g. system wide GHG targets) are used rather than sector specific. Technology agnostic measures are usually preferred, to promote the development of the most competitive options, and ensure that governments do not choose technologies with higher costs for society. However, due to the learning curve effect, some technologies that are not economically attractive in the early stages of deployment may deliver a lower long-term cost. This requires additional incentives to go beyond this "valley of death" region to be able to reach that long-term target [97].

For example, although electrolysis is a relatively well established technology, studies that find hydrogen from electrolysis to be competitive with conventional hydrogen production or even fossil fuel alternatives usually rely on reductions in cost resulting from significant scale-up of production (e.g. [91]), which most likely would only occur with strong government support. Similarly, for technologies at the R&D level, incentives need to be technology specific since this will determine the research strategy and priorities. In turn, this R&D can lead to cost and efficiency improvements, which will influence the prominence of the technology in energy scenarios. Experience from the power sector has shown that a mix of technology specific and technology neutral policies achieve the best results in promoting low carbon options [98].

Model-based scenario studies should model a full range of technology and policy assumptions. Ideally, sensitivity analysis would be used to understand the significance of different data uncertainties on scenario results. This analysis may also provide insights into the relative value of R&D for different technologies and sectors. Of course, sensitivity analyses can be expensive when applied to large, complex models, hence there is an argument for simpler models, with a more thorough treatment of data uncertainty [47]. Despite this, the models should not be simplified to the point where they no longer represent the energy system with sufficient accuracy, as this will result in unrealistic sensitivities, especially when non-linear effects are involved. The simplified model should only be used for sensitivity analysis and the more-detailed model used to explore interesting "corner" points identified in the analysis – to check that the analysis is correct.

As a minimum, studies should share the data assumptions that were made in their analysis but unfortunately even this is rare. The IEA H2FC Roadmap [29] and IIASA Global Energy Assessment [65] contain detailed descriptions of the technical and economic performance of most hydrogen technologies throughout the supply chain. However, as Figure 3-2 shows, several studies include hydrogen in their scenario results but little or no information at all is given on the data assumptions made (e.g. WEC [15], Shell [16]).

3.5 Conclusions

Energy systems are becoming more technologically diverse, spatially distributed and temporally variable. Consequently, there is an opportunity for new "flexibility" options, such as hydrogen, to play a role. In the authors' view, the greatest opportunities for hydrogen lie in the industrial and heavy-duty transport sectors, where hydrogen's high energy density and low greenhouse gas emissions could make it the preferred energy carrier. With the establishment of large-scale hydrogen production, transportation and storage infrastructure for these sectors, there will be many opportunities to use hydrogen for additional flexibility in other sectors, such as the power sector.

However, the exact role that new technologies such as hydrogen will have is unclear, and it is the purpose of energy scenarios to help to indicate what the role might be. In the authors' view, global energy scenarios, especially those based on energy system models, have been pessimistic with respect to hydrogen. This is beginning to change but coverage of hydrogen is still often restricted to a few main applications, such as mobility.

The main challenge for energy systems models is that many of the opportunities for new technologies such as hydrogen are in spaces that previously have not existed in energy systems, for example in energy storage (both at short and long time scales) and for sector-coupling. Energy systems models have traditionally not been good at representing the fine details, such as temporal variability. Capturing these details, whilst also encompassing the big picture of a long-term global energy transition is computationally and practically complex, and therefore a big challenge for the modelling community. Nonetheless, techniques are emerging to handle these complexities, and computational power is improving all the time, enabling more ambitious projects. We believe that overcoming these challenges will be necessary to determine with confidence the role that hydrogen should play in the future energy mix.

Meanwhile, if global energy scenarios are currently unable to represent all of the fine details and nuances of future energy systems, it is essential that they acknowledge this and do not present their scenario results with overconfidence. Much greater sharing of the methodologies and input assumptions behind energy scenarios is needed, so that the implications of the results can be correctly interpreted. Scenario developers should also constantly improve their practice, informed by findings from elsewhere. Numerous alternative approaches have been developed for exploring the role of new technologies in future energy systems, including qualitative scenarios and more detailed energy systems modelling at smaller scales. All of this research is valuable and should be taken into account with as much esteem as global energy scenarios.

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Chapter concluding remarks

In the concluding remarks to this chapter, the contributions of the article in the context of this thesis are discussed.

The perspective article includes an analysis of influential global energy scenarios, as well as a discussion of a range of other studies. The article provides some insights into the assumptions and modelling methods of the global scenarios, although as the article shows, the scenarios are often very opaque concerning their methods. Nonetheless, there is some value in comparing the results of the various scenarios, and understanding the "mainstream" views of influential institutions with respect to the energy transition, and hydrogen in particular.

Furthermore, the article illustrates the large variety of models considered "energy system models". Each of these has its own methods and scope, and differing models can give different answers to seemingly the same question. This emphasises the importance of a clearly defined scope, and ensuring the modelling tool and scenario design is correctly focussed on the research question.

The "best practice" guidelines prescribed in the article will be used directly to guide the modelling work carried out in the remainder of this thesis. With regard to model configuration, this will mean ensuring the model has sufficient spatial, temporal and technological detail, while remaining a manageable size. The model formulation must also be clearly presented (it can be found in each of the articles presented in this thesis). The scenarios that are modelled should also be carefully considered, including the appropriate technologies and sectors, and a variety of policy and economic scenarios. Using accurate input data assumptions, and being transparent with these data assumptions is also important.

One clarification to the article should be noted, which has been identified since it was published. In Figure 3-1, production of hydrogen from biomass can take place using either gasification or fermentation.

Chapter 4

The value of hydrogen and carbon capture, storage and utilisation: Insights from value chain optimisation

Chapter introductory remarks

This chapter is based on the research article published by Elsevier in Applied Energy. The publisher permits the re-use of the article in this thesis, provided that the journal is referenced as the original source. The article details are as follows:

> Christopher J. Quarton and Sheila Samsatli. The value of hydrogen and carbon capture, storage and utilisation: Insights from value chain optimisation. *Applied Energy*, 257:113936, 2020. https://doi.org/10.1016/j.apenergy.2019.113936

This chapter is the first of three chapters that present the modelling work of this thesis. The article in this chapter was the first major piece of modelling work that was undertaken for the thesis.

Chapters 2 and 3 have shown the need for high quality models to explore the role of hydrogen in energy systems. Chapter 2 showed that there is strong interest in power-to-gas and associated technologies, but the best ways to implement these technologies is not yet fully understood. Modelling can help to improve this understanding, but models are needed that have sufficient spatial, temporal and technological detail, whilst also incorporating the needs of the wider energy system. Chapter 3 furthered this argument, contending that many of the models underpinning influential global energy scenarios do not have sufficient detail, which may explain the limited contribution of hydrogen to the scenario results.

The article that is presented in this chapter introduces a model that does have many of the characteristics necessary to represent hydrogen more accurately. The model in question is the Value Web Model (VWM), and is introduced and described in detail in the article. The VWM was developed by S. Samsatli and N.J. Samsatli; the appropriate references are provided within the article. In the work for this chapter, some additions were made to the model, most notably by including a more detailed representation of CO_2, allowing for modelling of carbon capture, utilisation and storage (CCUS) technologies. All of the configurations made to the model are described in the article.

As the article argues, many hydrogen value chains are closely linked with CO_2 value chains. Therefore, a detailed representation of CO_2 is essential to ensure that hydrogen value chains are correctly modelled. For example, some hydrogen value chains, such as hydrogen production from fossil fuels, are directly dependent on CCUS technologies for decarbonisation. Meanwhile, accurate tracking of CO_2 emissions is essential for modelling all energy value chains in the context of decarbonisation.

In addition to introducing the VWM and describing the updates made in this work, the article in this chapter provides a review and discussion of the debate concerning CCUS and hydrogen technologies. A series of scenarios are also modelled, illustrating the capabilities of the model and exploring the potential of CCUS and hydrogen technologies for contributing decarbonisation and flexibility to the Great Britain energy system.

Following this introduction, an authorship declaration is provided, followed by the article as published in Applied Energy (although re-formatted for this thesis). The article includes its own reference list. Not all of the original article appendices are presented in this chapter, but a guide to where the contents of the original appendices can be found is provided at the end of the article. Finally, some concluding remarks are provided at the end of the chapter, including further discussion of the contribution of the article, and its relevance to this thesis.

Authorship declaration

<table>
<tr><td colspan="2">This declaration concerns the article entitled:
The value of hydrogen and carbon capture, storage and utilisation: Insights from value chain optimisation</td></tr>
<tr><td colspan="2">Publication status
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<tr><td colspan="2">Copyright status
I hold the copyright for this material ☐ Copyright is retained by the publisher, but I have been given permissions to replicate the material here ☒</td></tr>
<tr><td>Candidate's contribution to the paper</td><td>The candidate contributed to / considerably contributed to / predominantly executed the...
Formulation of ideas:
50% - S. Samsatli and I jointly conceptualised the study.
Design of methodology:
60% - S. Samsatli provided the Value Web Model for this project and we jointly developed the new CO_2 value chain representation in this chapter. I developed the initial scenarios to study, with support from S. Samsatli.
Experimental work:
95% - With some assistance from S. Samsatli, I assembled the model input data and carried out all of the model runs, post-processing and analysis. S. Samsatli suggested using factorial analysis, which I carried out.
Presentation of data in journal format:
80% - I structured and wrote the article, and designed all of the figures. S. Samsatli provided comments and contributions to the draft, made final edits to the manuscript for submission to the journal and helped address the reviewers' comments.</td></tr>
<tr><td>Statement from candidate</td><td>This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.</td></tr>
</table>

Signed		**Date**	16/11/2020

Article:

The value of hydrogen and carbon capture, storage and utilisation: Insights from value chain optimisation

Abstract

There is increasing interest in carbon capture, utilisation and storage (CCUS) and hydrogen-based technologies for decarbonising energy systems and providing flexibility. However, the overall value of these technologies is vigorously debated. Value chain optimisation can determine how carbon dioxide and hydrogen technologies will fit into existing value chains in the energy and chemicals sectors and how effectively they can assist in meeting climate change targets. This is the first study to model and optimise the integrated value chains for carbon dioxide and hydrogen, providing a whole-system assessment of the role of CCUS and hydrogen technologies within the energy system. The results show that there are opportunities for CCUS to decarbonise existing power generation capacity but long-term decarbonisation and flexibility can be achieved at lower cost through renewables and hydrogen storage. Methanol produced from carbon capture and utilisation (CCU) becomes profitable at a price range of £72–102/MWh, compared to a current market price of about £52/MWh. However, this remains well below existing prices for transport fuels, so there is an opportunity to displace existing fuel demands with CCU products. Nonetheless, the scope for decarbonisation from these CCU pathways is small. For investment in carbon capture and storage to become attractive, additional drivers such as decarbonisation of industry and negative emissions policies are required. The model and the insights presented in this paper will be valuable to policymakers and investors for assessing the potential value of the technologies considered and the policies required to incentivise their uptake.

Abbreviations: BECCS: Biomass Energy Carbon Capture and Storage; CAPEX: Capital expenditure; CCGT: Combined Cycle Gas Turbine; CGH2S: Compressed gas hydrogen storage; CCS: Carbon Capture and Storage; CCU: Carbon Capture and Utilisation; CCUS: Carbon Capture, Utilisation and Storage; CH_4: Methane; CHP: Combined Heat and Power; CO_2: Carbon dioxide; DACS: Direct Air (carbon) Capture and Storage; Elec: Electricity; EU ETS: European Union Emissions Trading Scheme; FT: Fischer-Tropsch; GB: Great Britain; H_2: Hydrogen; LHV: Lower Heating Value; MeOH: Methanol; MILP: Mixed Integer Linear Programming; NPV: Net Present Value; OPEX: Operating cost; PEM: Proton Exchange Membrane; RWGS: Reverse Water-Gas Shift; SMR: Steam Methane Reforming; tCO_2: Tonnes of Carbon dioxide; US-H2: Hydrogen underground storage; VWM: Value Web Model.

4.1 Introduction

Vast reductions in greenhouse gas emissions are required if the worst effects of climate change are to be prevented by keeping global temperature changes below 2°C or even 1.5°C [1, 2]. Primary energy use accounts for over 70% of global greenhouse gas emissions [1, 3], so our energy systems must be decarbonised. Additionally, there is an increasing need for low-carbon sources of flexibility for energy systems, where in the past systems have relied on fossil fuels to meet hourly, daily and seasonal demand variations, whether for heating, or in dispatchable power stations for electricity [4].

There is considerable interest in carbon capture and storage (CCS) for providing decarbonisation and flexibility to energy systems. Figure 4-1 shows the distribution of energy-based CO_2 emissions globally: almost half of these emissions arise from centralised heat and electricity production, well-suited to CO_2 capture. Further capturable emissions are available from industrial plants (both fuel combustion and process emissions). Fitting CO_2 capture to fossil fuel power plants could enable low-carbon, flexible electricity production. CCS solutions for "diffuse" emissions such as transport and buildings, which together make up 29% of energy-based emissions globally, are less obvious, although technologies such as Direct Air Capture and Storage (DACS) show interesting potential in this area [5]. Furthermore, technologies such as Biomass Energy CCS (BECCS) are gathering interest due to their potential to achieve net-negative emissions for the energy they deliver [5], although the wider environmental implications of biomass-based solutions must be considered carefully [6].

Beyond CCS, there is growing interest in alternative uses for captured CO_2, known as carbon capture and utilisation (CCU), that may enable emissions reductions whilst also delivering useful products and energy system flexibility. In CCU, rather than considering CO_2 emissions as an unwanted by-product, they are viewed as a resource for subsequent processes. CCU processes may involve use of CO_2 as an industrial feedstock, or conversion to synthetic fuels for use in energy systems. Hydrogen (H_2) is integral to many of these energy-based CCU pathways: for example, in Fischer-Tropsch synthesis, synthetic hydrocarbons are manufactured from CO_2 and hydrogen [7]. CCU has the potential to add economic incentive to CO_2 capture by creating a marketable final product from the CO_2 [8]. However, the potential of CCU for large-scale decarbonisation has been questioned [9].

Many other technologies exist that offer decarbonisation and flexibility potential without involving CO_2 capture. In the context of CO_2 capture, utilisation and storage (CCUS), it is also relevant to consider hydrogen technologies such as electrolysis and hydrogen storage [10]. With these technologies, it is possible to imagine a flexible energy system with no reliance on hydrocarbons or CO_2 at all [11, 12].

There is strong debate concerning the relative value of these various technologies for supporting a low-carbon, flexible energy system. For example, studies such as Mac Dowell et al. [9] and Bruhn et al. [13] have compared the merits of CCU and CCS, whilst others such as Ball and Weeda [14] and McPherson et al. [15] have assessed the potential of a future "hydrogen economy". However, these studies typically consider the technologies in isolation, perhaps not in their optimal configurations, and without considering the implications for the wider environment, energy system, and economy.

The environmental impacts of these processes are complex, so require comprehensive analysis. Life cycle analysis (LCA) is valuable in this regard. Cuéllar-Franca and Azapagic [16] used LCA to assess CCS and CCU, whilst Parra et al. [17] performed LCA on P2G. Both studies found several cases in which the processes being studied were less environmentally favourable than conventional fossil fuel pathways. Assessing the environmental impacts of a single process can be treacherous, as decisions regarding where to apportion environmental "burden" may lead to a different result than when considering the system as a whole [18].

Some energy systems models have been applied to CCUS and hydrogen, attempting to quantify the system-level economic and environmental costs and benefits. For example, Blanco et al. [19] assessed the role of hydrogen in the EU using the JRC-EU-TIMES model, with various applications for the hydrogen including in CCU. Meanwhile Antenucci and Sansavini [20] assessed the potential of power-to-methane for recycling CO_2 through a coupled electricity planning and gas network simulation model. However, these models can still have system boundaries that do not account for the full impacts of the processes being modelled. Furthermore, these models typically lack the spatial, temporal and technological detail required to represent the interactions between technologies that may lead to different business cases or environmental impacts [21].

Value chain modelling and optimisation is a valuable method for representing the detailed interactions of energy processes, whilst also capturing the overall system effects. Value chain modelling determines the most effective pathways for converting low-value primary resources and raw materials through a network of technologies to produce final products and services with high economic, social or environmental value [22]. Applying this methodology to CCUS and hydrogen processes enables the comparison of CCS and CCU, as well as alternative decarbonisation strategies, in their optimal configuration, taking into account CO_2 capture and purification, sourcing the energy and feedstocks (including hydrogen) required for the processes, logistics, and delivery of final products

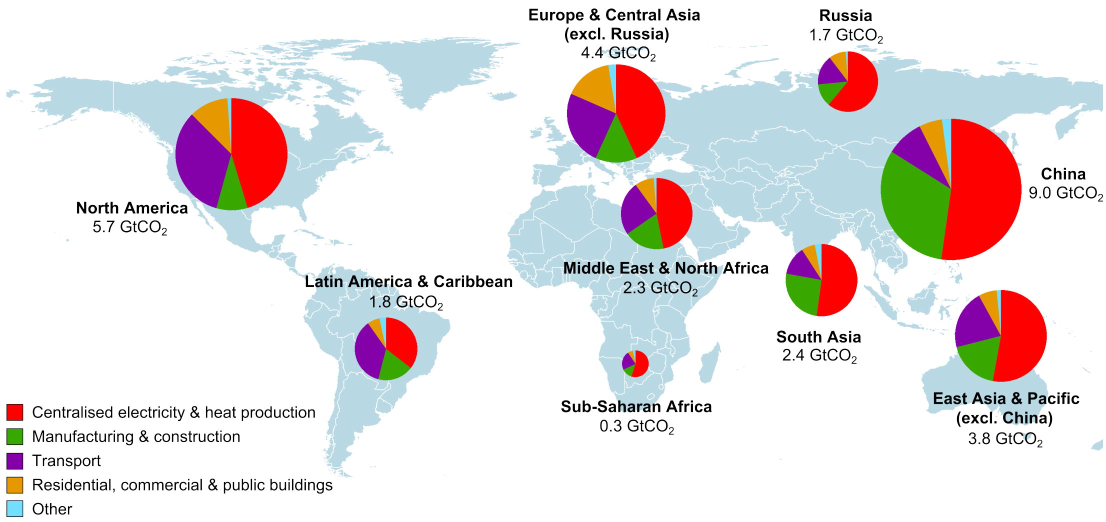


Figure 4-1: **Global CO_2 emissions from fuel combustion in 2014.** Data from the IEA [27] and the Carbon Dioxide Information Analysis Center [28], accessed using the World Bank DataBank [29]. Graphic inspired by Scott et al. [30].

and energy services to customers. Value chain modelling and optimisation has been applied to many fields, including hydrogen value chains. For example Samsatli and co-workers have modelled hydrogen value chains for multiple applications in the UK [23, 24] and Welder et al. [25] modelled similar scenarios in Germany. Using the BeWhere model, Mesfun et al. [26] investigated the potential for hydrogen in the Alpine region, including using hydrogen in CCU, however they did not model the CO_2 value chain itself. Therefore, this paper is the first to apply value-chain optimisation to integrated CO_2 and hydrogen value chains, providing a whole-system assessment of the potential that CCUS and hydrogen technologies have for delivering decarbonisation and flexibility.

In Section 4.2, the key arguments in the CCUS debate are discussed. Section 4.3 provides an overview of hydrogen and CO_2 value chains. In Section 4.4, the comprehensive value chain optimisation model that was developed for this study is presented. Section 4.5 describes the scenarios that were modelled in this study. Great Britain (GB) was used as an exemplar of an energy system that faces decarbonisation and flexibility challenges. A number of different economic and policy assumptions were modelled in order to quantify and compare the value of CCS, CCU and hydrogen technologies over the next 40 years. Finally, Section 4.6 presents the results of these scenarios and discusses their implications.

4.2 The CCUS debate

There is strong debate regarding the relative merits of CCS and CCU for helping to enable a low carbon energy transition. However, considering these technologies as direct competitors can be problematic, as they often serve different purposes [13]. Furthermore, it is useful to consider hydrogen value chains in this debate, as they are both intrinsic to CCU, and also potential competitors. The discussion surrounding the technologies can be separated into six themes.

Scale. Assuming that CCUS technologies must sequester up to 160 $GtCO_2$ globally by 2050 in order to contribute to the 2050 2°C target, Mac Dowell et al. [9] argue that this would only require one sixth of the storage capacity of depleted oil and gas reservoirs and that there is considerably more capacity still in deep saline aquifers. They argue that the projected market size for CCU, however, allows for less than 3% of the 160 $GtCO_2$ to be sequestered for a significant duration. Nonetheless, there is some scope for demands for CCU products to grow in the future, for example if methanol were adopted at scale in the transport sector [31], and even if CCU is not capable of utilising all possible emissions, this is not a reason to prevent its uptake altogether.

Sustainability. CCS is inherently an unsustainable process: whilst the capacity for storage might be large, it is still finite. Additionally, since no CCS facilities have been operated for a long duration, the long-term effects are still uncertain [32]. Meanwhile performing environmental assessments of CCU is strewn with pitfalls, as all of the impacts in the system must be correclty accounted for, environmental "burdens" apportioned appropriately [18]. In many CCU processes, CO_2 is only sequestered temporarily, being re-released into the atmosphere when the product is used. While CCU products may be able to replace fossil fuel usage to some extent, in some cases the life-cycle global warming potential of CCU products has been found to be higher than that of the fossil-fuel equivalent [16]. Nonetheless, there are scenarios in which the CO_2 emissions from the CCU product could be re-captured and re-utilised, creating a sustainable CO_2 cycle [33].

Economics and efficiency. CCU is capable of producing a product with an economic value, independent of any environmental benefits [8]. CCS meanwhile is merely an emissions mitigation strategy that without regulatory support has no clear business case [30]. Perhaps, there is potential to build CCU and CCS projects in unison, where CCU can provide some financial support to CCS [34]. Whilst both CCS and CCU already have examples of commercial operations, it is also difficult to determine how the economics of each would change if the scale of the operations were vastly increased

[35, 36]. Despite the apparent economic incentive of CCU, concerns have been raised with regard to the efficiency of the processes, due to the levels of energy input required in both the capture and utilisation stages [30]. Of course, CCS processes also require energy inputs in addition to the capture processes, for example for compression and transportation.

Flexibility. Traditionally, electricity systems have relied on fossil fuel fired generators such as CCGTs to provide system flexibility and stability, both through the spinning reserve they provide and the capability to ramp up or down generation in line with electricity demand. Some argue that in electricity systems with increasing penetrations of variable renewable sources such as wind and solar, these fossil fuel generation options will be even more essential [37]. If this is the case, then carbon capture technologies may be required to minimise the emissions of these generators. Furthermore, although the CCU processes are relatively energy intensive, it is possible that these energy requirements could be used to balance overall system supplies and demands, e.g. by using "power-to-liquids" processes [7]. For example, processes that utilise hydrogen as a feedstock can be used for load balancing if the hydrogen is produced from electrolysis, which can be ramped up and down in line with a variable electricity supply, and has been shown to be capable of providing frequency response services to electricity grids [38]. The hydrogen can be stored, then supplied at a constant rate to CCU processes. Moreover, the final products of CCU are often relatively easy to store, and could be used as fuels on the occasions when demand exceeds supply [33].

Infrastructure. A major challenge for CCS is that it requires a transport infrastructure connecting capture and storage facilities, particularly as this leads to a "chicken and egg problem" where capture plants, storage facilities and transport infrastructures all need to be invested in before any benefits of CCS are achieved [30]. This would require significant start-up investments and collaboration between all stakeholders. It is argued that if CCU were implemented effectively, utilisation facilities could be located near to large sources of CO_2 from capture plants, minimising the need for a costly CO_2 transport network [33]. However, this would also be likely to need significant stakeholder collaboration and encouragement to implement. Furthermore, CCU relies on additional feedstocks beyond CO_2 that will have their own production, distribution and storage requirements. Hydrogen, for example, whether used for CCU or other applications, requires a production infrastructure. "Power-to-gas" hydrogen production requires both electrolysers and sufficient (renewable) electricity production to power the process [10].

Diversification. Energy systems operators will look to diversify their sources of energy to ensure supply security. CCU could assist this through the production of a range of fuels that do not rely on specific natural resources (such as fossil fuels). Some argue meanwhile that CCS is only an enabling technology for the continuation of the fossil fuel industry, where supply security issues will only worsen over time [13], although this does not allow for the growing interest in BECCS.

Mathematical modelling can be used to help understand the issues discussed above and take a systematic account of the uncertainties associated with them. Furthermore, to ensure that CO_2 and hydrogen technologies are implemented in a manner that brings the greatest overall system benefit, a holistic approach is required. Policy-makers will need to identify the combination of technologies and networks that best satisfies economic, environmental and social objectives in order to devise suitable policy instruments (e.g. incentives, taxes, etc.). Value chain modelling and optimisation is a valuable tool that can examine these issues, at various scales from regional to national and trans-national scales, including how CO_2 and hydrogen technologies will fit into existing value chains in the energy and chemicals sectors and how effective they will be in helping to meet climate change targets.

4.3 Overview of hydrogen and CO_2 value chains

Many hydrogen and CO_2 technologies exist, and can be configured in various ways to create different value chains. In this section, the main technologies are described. Costs are provided in UK pounds sterling (£), but can be converted to US dollars at the 2018 average exchange rate of £1 = $1.34 [39].

4.3.1 Hydrogen value chains

The following subsections describe the key components of a hydrogen value chain.

4.3.1.1 Hydrogen production

Conventionally, hydrogen is produced from reforming natural gas (e.g. steam methane reforming), or gasification of coal, oil or biomass feedstocks [40]. Currently, around 95% of hydrogen is produced from fossil fuels [41]. These processes are well established, so have relatively low costs and energy penalties. For example, through steam methane reforming (SMR), hydrogen can be produced for around £28-33 /$\mathrm{MWh_{H_2\text{-}LHV}}$, with an efficiency of $76\%_{\mathrm{LHV}}$ (1.3 $\mathrm{MWh_{CH_4\text{-}LHV}}$ per $\mathrm{MWh_{H_2\text{-}LHV}}$)[42, 43]. In the modelling carried out in this study, SMR was selected as the fossil-based technology for hydrogen production, due to its high level of development and the large, established gas industry in the UK. However, to produce low-carbon hydrogen from fossil fuels, CCS is required, which adds significantly to the cost and energy penalty. For example, with a CO_2 capture rate of 90%, SMR costs may increase to around £48/$MWh_{H_2\text{-}LHV}$ with an efficiency of 69%$_{LHV}$ (1.4 $MWh_{CH_4\text{-}LHV}$ per $MWh_{H_2\text{-}LHV}$) [42].

Alternatively, there is growing interest in power-to-gas for hydrogen production [10, 11, 44]. State-of-the-art PEM or alkaline electrolysers have a system efficiency of around 60%$_{LHV}$ (1.7 MWh_{Elec} per $MWh_{H_2\text{-}LHV}$) [45]. Arguments for power-to-gas often rely on the availability of cheap excess electricity [44], and consequently cost estimates vary widely. The other major challenge for power-to-gas is scalability, with the largest power-to-gas projects in operation today being only a few megawatts in size [44].

4.3.1.2 Hydrogen storage and conversion

Hydrogen can be stored underground in geological formations including salt caverns, saline aquifers and depleted oil and gas fields [46]. Cost estimates for underground hydrogen storage depend on the geological formation and the operating regime, but capital costs for salt cavern storage are in the region of £70-250 per MWh of hydrogen storage capacity [47, 48]. Energy losses for underground hydrogen storage are low, arising predominantly from the compression energy requirements [48]. Hydrogen can also be stored in purpose-built pressure vessels. In this study, both underground (salt cavern) and above ground (pressure vessel) storage technologies were modelled.

Finally, hydrogen must be converted into its final useful form. This might be through CCU, as described in Section 4.3.2.3. Alternatively, hydrogen can be used for heating, similarly to natural gas, provided that the infrastructure (boilers and distribution infrastructure) is in place [49, 48]. Hydrogen can be converted to electricity, either through turbines or fuel cells [41, 50]. Due to relatively low conversion efficiencies for power-to-hydrogen and hydrogen-to-power, the overall performance of hydrogen energy (i.e. electricity) storage is low. For example, hydrogen power-to-power pathways may have round-trip efficiencies below 30% [50].

4.3.2 CO_2 value chains

This section describes the key components of a CO_2 value chain: capture, transportation, storage and utilisation of CO_2.

4.3.2.1 CO_2 capture and transportation

CO_2 capture can be carried out pre-combustion, post-combustion, or through oxy-fuel combustion [51]. Post-combustion capture through chemical absorption, for example amine scrubbing, is the most established technology and is well suited to capturing CO_2 from flue gases, e.g. from fossil power stations [52]. Rubin et al. suggest that for a CO_2 capture rate of 88%, a combined cycle gas turbine (CCGT) plant will require an additional 13-18% energy input for the same energy output, implying an energy penalty of around 870-1030 kWh of natural gas feedstock per tonne of CO_2 captured [53]. The additional CCGT plant cost would be £32-85 per tonne of CO_2 captured [53]. Achieving higher capture rates becomes increasingly expensive [51].

CO_2 transportation by pipeline is well established, capable of transportation onshore and to offshore wells [52]. Costs of transportation by pipeline are estimated to be around £2.50 per tonne of CO_2 per 100 km onshore, and £2.90-4.40 per tonne of CO_2 per 100 km offshore, depending on the pipeline length [54]. Energy requirements are in the region of 1.3-4.5 kWh per tonne of CO_2 for each compression station (which are required every 100-200 km) [55]. CO_2 transport by ship is also a possibility [54].

4.3.2.2 CO_2 storage

CO_2 can be stored underground in geological formations [51]. Globally there is thought to be capacity for around 1,000 $GtCO_2$ in depleted oil and gas reservoirs, and up to 10,000 $GtCO_2$ in deep saline aquifers [9]. The processes for CO_2 storage are well understood, with several projects already injecting CO_2 into depleted oil and gas reservoirs to enhance hydrocarbon extraction (Enhanced Oil Recovery) [51].

Estimates for CO_2 storage costs have a large range, predominantly due to variations in the suitability of different sites. For offshore depleted oil and gas wells, the Zero Emissions Platform estimates costs of £2-14 per tonne of CO_2 stored [56]. Storage in offshore saline aquifers may cost £6-20 per tonne of CO_2 [56]. In this study, CO_2 storage was assumed to be in depleted oil and gas wells, in four suitable offshore locations around the UK [57].

4.3.2.3 CO_2 utilisation

CO_2 utilisation encompasses a range of possible uses for captured CO_2, including as a chemical feedstock, mineral carbonation, and direct usage (e.g. in the food and drink industry) [8, 16]. CO_2 utilisation as a chemical feedstock to produce synthetic fuels is the focus of this paper, due to the potential to re-use these fuels as energy vectors. Various fuels can be synthesised through CO_2 utilisation [22]: below, some of the more mature CCU value chains are described.

Liquid hydrocarbons such as diesel and petrol can be manufactured from syngas through Fischer-Tropsch synthesis [22]. For Fischer-Tropsch to be used for CO_2 utilisation, captured CO_2 must first be converted into syngas using hydrogen. This can be done using the Reverse Water-Gas Shift (RWGS) reaction, where CO_2 and hydrogen are reacted at high temperature to produce carbon monoxide and water [22]. Alternatively, CO_2 and steam can be fed into a high temperature (solid oxide) electrolyser to produce hydrogen and carbon monoxide, as demonstrated by Sunfire at a plant in Germany [58]. Electricity requirements for the complete Fischer-Tropsch process (including for hydrogen production from electrolysis and other process requirements) are around 1.6-2.1 MWh_{Elec} per MWh_{LHV} of hydrocarbons produced [58, 59]. CO_2 utilisation is 0.43-0.56 tCO_2 per MWh_{LHV}.

An alternative CCU value chain is methanol production. Methanol is already used widely in the chemical industry and has potential as a fuel, e.g. in the transport sector [31]. Methanol can either be produced in a two-step process involving RWGS followed by methanol synthesis from syngas or produced from direct hydrogenation of CO_2 [60]. There is growing interest in "power-to-methanol", where hydrogen is produced from electrolysis and combined with captured CO_2. The George Olah plant in Iceland produces approximately 22,000 MWh of methanol per year through this process [22]. Based on modelling of a similar plant by Pérez-Fortes et al., the process would have a total electricity demand (including for electrolysis) of 2.0 MWh_{Elec} per MWh_{LHV} of methanol produced, utilising 0.22 tCO_2 per MWh_{LHV}[61].

Finally, captured CO_2 can be combined with hydrogen to produce methane through methanation. Most commonly, this process is carried out chemically, using the Sabatier process [22], but it is also possible to use biological methanation [10]. When the hydrogen is produced from electrolysis, this process is referred to as "power-to-methane" or sometimes "power-to-gas". In this work, "power-to-gas" is used to describe hydrogen production from electrolysis (as discussed in Section 4.3.1.1); the full process of electrolysis and methanation is named "power-to-methane". Depending on the CO_2 source of CO_2, power-to-methane could be a fossil-free alternative to natural gas, and has some advantages compared to power-to-hydrogen due to the availability of existing natural gas infrastructure. Several pilot plants use power-to-methane to convert electricity (e.g. from excess renewables) into methane that can be injected into the gas grid [44]. Power-to-methane has an overall efficiency of around $52\%_{\mathrm{LHV}}$ (1.9 $\mathrm{MWh_{Elec}}$ per $\mathrm{MWh_{CH_4\text{-}LHV}}$) [10], utilising 0.19 tCO_2 per $\mathrm{MWh_{CH_4\text{-}LHV}}$ [62].

4.4 Integrated value chain optimisation

The Value Web Model (VWM) was developed to optimise the integrated value chains for CCS, CCU and hydrogen in order to determine their roles in decarbonising an energy system over a 40 year period. The VWM is a value chain optimisation model, which was originally developed by Samsatli and Samsatli [63] and has been extended and configured for CO_2 and hydrogen value chains in this work. The VWM is a mixed-integer linear programming (MILP) model, which can represent interconnected pathways for converting primary resources (e.g. natural gas and wind) to final products and services (e.g. electricity and heat), through various technologies that convert, store and transport resources. The optimisation determines the system design (e.g. where and when to invest in technologies and infrastructures) and the operating strategy for this system in order to optimise an objective function, which may include system costs, environmental impacts, and other indicators. Space and time are both explicitly represented in the VWM, in order to capture the spatial distribution of primary resource availability and demands for energy and products as well as their time-varying nature [64]. Space is represented by a discrete set of zones and time is represented on four levels of granularity: hourly intervals for fast dynamics associated with storage and intermittent renewables (e.g. wind), day types to represent different days of the week, seasons and yearly planning periods.

Pathways are represented by a series of resources and technologies. Resources represent any type of material or energy involved in the pathway from primary resources to end products and energy vectors. Different technology types are included that can: (1) convert one or more resources to one or more other resources (e.g. a gas-fired CCGT that converts natural gas to electricity), (2) transport resources between zones or (3) store resources. Complex interconnected, linear and circular pathways can be constructed [65] by correctly defining resources and the technologies that inter-convert all of the resources.

The pathways can be represented graphically, as in Figure 4-2, which shows the value web representation for the CCUS and hydrogen value chains considered in this paper. The resources are represented by circles, some of which have demands that must always be met (grey circles in the diagram) and those that have demands that may optionally be met, if it is profitable to do so (striped circles). The rectangles represent the "con-

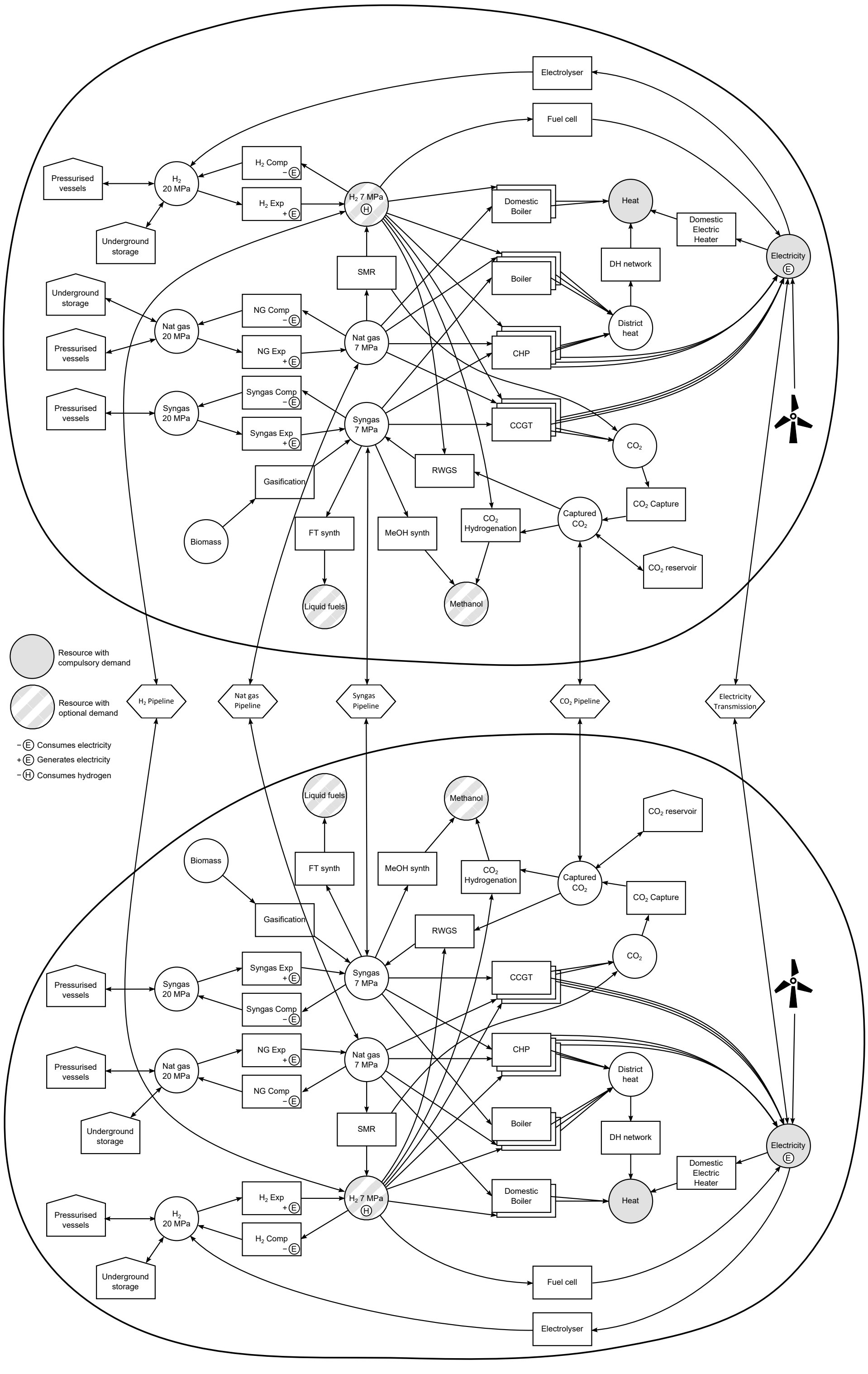


Figure 4-2: **Superstructure of the integrated hydrogen and CO_2 value chains in the value web model.** The diagram shows the potential value chain pathways for two representative zones only. The model determines what pathways are used in each zone to maximise net present value.

version" technologies, which convert one set of resources to another set, as indicated by the arrows linking the resources to the technologies (to avoid too many crossed arrows, some links are indicated by a circle enclosed within the technology, with a + indicating that that resource is produced by the technology and a − indicating that the resource is consumed by the technology). Storage technologies are represented by pentagons with double-headed arrows (indicating flow in either direction for charging and discharging) connecting the stored resource. Transport technologies are represented by hexagons connected by double-headed arrows connected to the transported resource.

Overall, the diagram shows two typical zones in the problem (of which there may be many 10s or 100s of zones needed to represent the full area being considered). The transport technologies move resources from one zone to another, as shown by the hexagons. Within each zone the possible energy pathways are shown. Considering the zone at the bottom of the diagram (the one at the top is a mirror image), the three primary resources are: natural gas ("Nat gas 7 MPa") at the centre of the value web; biomass at the top left; and wind, represented by the wind turbine symbol on the right. When wind turbines are installed in the zone, electricity can be generated as shown by the arrow pointing to the Electricity resource on the right, which is grey to indicate there are demands for it. Below and to the right of the "Nat gas 7 MPa" resource is the wind/hydrogen/natural gas/heat/electricity value web: natural gas can be converted to heat and/or power via CCGT, CHP, boiler (industrial/district scale) and domestic boiler technologies. Natural gas can be converted to hydrogen, which has optional demands, using the SMR technology and hydrogen can also be produced from electricity using the electrolyser technology, though at a higher pressure of 20 MPa. Hydrogen can also be used to generate electricity via the fuel cell technology.

The CCUS value web is shown above the "Nat gas 7 MPa" resource: syngas can be produced by gasification of biomass or by the RWGS (reverse water-gas-shift) technology, which reacts hydrogen with captured CO_2. The syngas can then be converted to liquid fuels in the FT synthesis ("FT synth") technology or to methanol via the methanol synthesis ("MeOH synth") technology. Methanol can also be produced from hydrogen via the "CO_2 hydrogenation" technology, which also utilises captured CO_2. CO_2 can only be captured from certain technologies, e.g. SMR and CCGT, that are at a large enough scale to be equipped with a CO_2 capture technology. Any captured CO_2 that is not utilised by "utilisation" technologies must be stored in a CO_2 reservoir (i.e. it cannot be captured and then released to atmosphere). The CO_2 emissions from all technologies, including those that can have their CO_2 captured, are tracked through their operating impacts. Any CO_2 that is captured is then offset against these emissions as described in section 4.4.1.5.

Storage of resources other than CO_2 is possible: on the left of the value web can be seen the storage technologies for hydrogen, natural gas and syngas. These gases are stored at a pressure of 20 MPa and therefore need to be compressed from their normal pressures of 7 MPa (the maximum pressure in transmission pipelines) up to this level, which requires some electricity. Conversely, some energy can be recovered when the resources are taken out of storage by using a turbine to generate some electricity. In Figure 4-2, technologies ending in "Comp" or "Exp" represent compressors and expanders, respectively.

Finally, the transport technologies are shown as hexagons between the two typical zones. Pipelines can be built to transmit hydrogen, syngas or CO_2 between any pair of adjacent zones. Existing pipelines and electricity transmission lines can used to transport natural gas and power, respectively, as well as there being the possibility of extending/reinforcing these networks where necessary.

4.4.1 Model formulation

The Value Web Model consists of a large number of constraints governing the flows of resources, management of technologies (investments, operation etc.), satisfaction of demands and socio-enviro-techno-economic constraints, which are all solved simultaneously. The key constraints required to understand the model behaviour are presented here, and the nomenclature is included in Appendix B. The complete mathematical formulation of the model can be found in the supplementary material*.

4.4.1.1 Objective function

The objective function in the Value Web Model is the minimisation of a weighted sum of all of the "impacts" of the value chain:

$$\begin{aligned} Z = \sum_{iy} \omega_i (\mathscr{I}^{\mathrm{W}}_{iy} + \mathscr{I}^{\mathrm{P}}_{iy} + \mathscr{I}^{\mathrm{S}}_{iy} + \mathscr{I}^{\mathrm{Q}}_{iy} + \mathscr{I}^{\mathrm{w}}_{iy} + \mathscr{I}^{\mathrm{fp}}_{iy} \\ + \mathscr{I}^{\mathrm{fs}}_{iy} + \mathscr{I}^{\mathrm{fq}}_{iy} + \mathscr{I}^{\mathrm{vp}}_{iy} + \mathscr{I}^{\mathrm{vs}}_{iy} + \mathscr{I}^{\mathrm{vq}}_{iy} + \mathscr{I}^{\mathrm{m}}_{iy} + \mathscr{I}^{\mathrm{x}}_{iy} \\ + \mathscr{I}^{\mathrm{U}}_{iy} + \mathscr{I}^{\mathrm{IET}}_{iy} - \mathscr{I}^{\mathrm{CUS}}_{iy} - \mathscr{I}^{\mathrm{Rev}}_{iy}) - \epsilon \sum_{y} E^{\mathrm{TOT}}_{y} n^{\mathrm{yy}}_{y} \end{aligned} \quad (4.1)$$

*The original article appendices and supplementary material are not included in this thesis. A full model nomenclature is provided in Appendix A of this thesis.

Each impact, $\mathscr{I}_{iy}$, is the value of one of a number of key performance indicators, i, such as costs or CO_2 emissions, in yearly planning interval y for one of the activities in the value chain, signified by the superscript symbol. These include: capital investments into wind turbines (W), production technologies (P), storage technologies (S) and transport infrastructures (Q); fixed and variable operating impacts for wind turbines and the three different types of technology (w, fp, fs, fq, vp, vs, vq); imports and exports (m and x); utilisation of primary resources (U); CO_2 emissions and credits (IET and CUS); and revenues from satisfying demands for energy and fuels (Rev) – these are described in the subsequent subsections. The weighting factors ω_i represent the relative contribution of each key performance indicator to the weighted-sum objective function. Economic impacts are discounted back to present value based on a discount rate. The final term in the objective function is the total annual energy production in each planning period, E_y^{TOT}, so that if $\omega_i = 0\ \forall i$ and $\epsilon = 1$ then the objective function is to maximise energy production.

4.4.1.2 Resource balance

The resource balance is essentially an energy balance that applies to all resources, r, in all zones, z, and at all times: every hourly interval, h, of every day type, d, of each week in every season, t, and yearly planning interval, y. The flows of resource into each zone must be equal to the flows out as follows:

$$\begin{aligned} &U_{rzhdty} + M_{rzhdty} + P_{rzhdty} + S_{rzhdty} + Q_{rzhdty} \\ &\qquad = D^{\mathrm{comp}}_{rzhdty} + D^{\mathrm{sat}}_{rzhdty} + X_{rzhdty} + E_{rzhdty} \\ &\qquad\qquad \forall r \in \mathbb{R},\ z \in \mathbb{Z},\ h \in \mathbb{H},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y} \end{aligned} \tag{4.2}$$

U_{rzhdty} is the rate of utilisation of naturally available resource r in zone z during hour h, day type d, season t and planning period y; P_{rzhdty} is resource production by conversion technologies; S_{rzhdty} is the net "production" of resources due to the operation of storage technologies (positive if resource is used from storage and negative if resource is stored); Q_{rzhdty} is the net transport rate of resource into the zone; M_{rzhdty} and X_{rzhdty} are the rates of resource import and export; $D^{\mathrm{comp}}_{rzhdty}$ and $D^{\mathrm{sat}}_{rzhdty}$ are the resource demands; and E_{rzhdty} is the excess resource production. Depending on the resource, any excess production can be curtailed for free or must be disposed of at an expense.

4.4.1.3 Utilisation of primary resources

Certain primary resources will be available in many or all zones and can be harvested if desirable. Three such resources are modelled in this study: natural gas, wind and biomass.

Natural gas availability, $u^{\max}_{\text{NG},zhdty}$, is given as an input to the model with data obtained from the National Grid's gas transmission operational data [66]. This maximum availability is used to limit the amount of resources that can be utilised:

$$U_{rzhdty} \leq u^{\max}_{rzhdty} \qquad \forall r \in \mathbb{R} - \mathbb{C},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.3}$$

which applies to all resources other than biomass, represented by the set $\mathbb{C}$, which is treated slightly differently.

For wind, the maximum amount of electricity that can be generated and utilised is given by the number and types of wind turbines installed in each zone, their characteristics and the wind speed:

$$u^{\max}_{\text{Elec},zhdty} = \frac{\rho^{\text{air}}}{2 \times 10^6} \sum_{w} \left(\eta_w \left[N^{\text{W}}_{wzy} \pi \left(R^{\text{W}}_w \right)^2 + N^{\text{EW}}_{wzy} \pi \left(R^{\text{EW}}_w \right)^2 \right] \tilde{v}^3_{wzhdty} \right)$$
$$\forall z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.4}$$

where ρ^{air} is the density of air; η_w is the efficiency of wind turbine type w (which in this study includes onshore and offshore turbines); N^{W}_{wzy} and N^{EW}_{wzy} are the number of new and existing wind turbines in operation; R^{W}_w and R^{EW}_w are the radii of turbine rotors; and $\tilde{v}_{wzhdty}$ is the "effective" wind speed, which accounts for the cut-in, cut-out and rated wind speeds of the turbines and gives the correct electricity generation rate based on the actual wind speed (which is an input to the model) and the turbine rating. Installation of new wind turbines depends on the availability of suitable land (or seabed) area, $A^{\text{W},\max}_{wzy}$, which is determined using a Geographic Information System (GIS) site-suitability analysis [24]. Assuming that new wind turbines will be erected on a hexagonal grid with a spacing of five rotor diameters, the number that can be installed in any zone is restricted by:

$$2\sqrt{3} \left(5R^{\text{W}}_w \right)^2 N^{\text{W}}_{wzy} \leq A^{\text{W},\max}_{wzy} \qquad \forall w \in \mathbb{W},\, z \in \mathbb{Z},\, y \in \mathbb{Y} \tag{4.5}$$

As biomass is seasonal and also depends on the area planted, the availability of biomass depends only on the season and is determined by the model, which chooses how much area to allocate to each crop, c. The availability is the product of the seasonal yield, Y^{Bio}_{czty}, and the area, A^{Bio}_{czy}, of land allocated to cultivating and harvesting each crop. The harvested biomass from each season is stored and can be utilised at any time during that season, provided the total utilisation over the season does not exceed the availability:

$$\sum_{hd} U_{czhdty} n^{\text{hd}}_h n^{\text{dw}}_d n^{\text{wt}}_t \leq A^{\text{Bio}}_{czy} Y^{\text{Bio}}_{czty} \qquad \forall c \in \mathbb{C} \subseteq \mathbb{R},\, z \in \mathbb{Z},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.6}$$

where n^{hd}_h, n^{dw}_d, and n^{wt}_t define the length of each hourly interval h, number of each day type d in each week, and the number of weeks in season t. Thus, the sum on the left-hand side of equation 4.6 gives the total utilisation in each season t.

The area of land that is suitable for biomass production, $A^{\text{Bio,max}}_{zy}$, is also obtained via a GIS site-suitability analysis, based on a number of constraints such as slope, elevation, topsoil organic carbon and other socio-political restrictions [67]. This is used to constrain the amount of area that can be allocated to biomass production, at local and national levels:

$$\sum_{c} A^{\text{Bio}}_{czy} \leq f^{\text{loc}}_{zy} A^{\text{Bio,max}}_{zy} \qquad \forall z \in \mathbb{Z},\, y \in \mathbb{Y} \tag{4.7}$$

$$\sum_{cz} A^{\text{Bio}}_{czy} \leq f^{\text{nat}}_{y} \sum_{z} A^{\text{Bio,max}}_{zy} \qquad \forall y \in \mathbb{Y} \tag{4.8}$$

where f^{loc}_{zy} is the fraction of suitable area that can be allocated to biomass production in zone z and f^{nat}_{y} is the fraction of the total suitable area that can be allocated.

The impacts associated with utilising resources are included in the objective function through the variables $\mathscr{I}^{\text{U}}_{iy}$, which include impacts for planting and harvesting biomass, and impacts for extracting natural gas and other resources. The capital and operating impacts of wind turbines are also included: $\mathscr{I}^{\text{W}}_{iy}$ and $\mathscr{I}^{\text{w}}_{iy}$, respectively. All of these impacts are defined in the supplementary material†.

† The article supplementary material is not provided in this thesis, but can be found with the original article.

4.4.1.4 Conversion technologies

Conversion technologies take resources as inputs and produce other resources as outputs. The net rate of production of a resource r by a conversion technology p is defined as follows:

$$P_{rzhdty} = \sum_p \mathscr{P}_{pzhdty}\alpha_{rpy} \qquad \forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.9}$$

where $\mathscr{P}_{pzhdty}$ is the operating rate of all technologies of type p, in zone z, at time $hdty$. The conversion factor α_{rpy} defines the rate at which resource r is consumed/produced by technology p per unit rate of operation of the technology – it is positive if resource r is produced by technology p and negative if it is consumed.

The operating rate of each technology is limited by the maximum rate of a single technology and the number of technologies present in each zone, as well as by a part-load constraint, as follows:

$$\begin{aligned} p_p^{\min} N_{pzy}^{\mathrm{PC}} \leq \mathscr{P}_{pzhdty} \leq p_p^{\max} N_{pzy}^{\mathrm{PC}} & \\ \forall p \in \mathbb{P},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} & \end{aligned} \tag{4.10}$$

The total number of technologies installed in zone z in planning period y, N_{pzy}^{PC}, is tracked based on the number of pre-existing technologies, N_{pz}^{EPC}, number of new technologies installed, NI_{pzy}^{PC}, and number of new technologies and pre-existing technologies retired (NR_{pzy}^{PC} and NR_{pzy}^{EPC}):

$$N_{pzy}^{\mathrm{PC}} = \begin{cases} N_{pz}^{\mathrm{EPC}} + NI_{pzy}^{\mathrm{PC}} - NR_{pzy}^{\mathrm{PC}} & \forall p \in \mathbb{P}^{\mathrm{C}},\, z \in \mathbb{Z},\, y = 1 \\ N_{pz,y-1}^{\mathrm{PC}} + NI_{pzy}^{\mathrm{PC}} - NR_{pzy}^{\mathrm{PC}} - NR_{pzy}^{\mathrm{EPC}} & \forall p \in \mathbb{P}^{\mathrm{C}},\, z \in \mathbb{Z},\, y > 1 \end{cases} \tag{4.11}$$

A constraint is also included to limit the number of commercial technologies that can be built in a given planning period:

$$\sum_z NI_{pzy}^{\mathrm{PC}} \leq BR_{py} \qquad \forall p \in \mathbb{P}^{\mathrm{C}},\, y \in \mathbb{Y} \tag{4.12}$$

where BR_{py} is the maximum allowable build rate of technology p in planning period

y. The impacts of investment in and operation of conversion technologies are a major contributor to the objective function. The total net present capital impact for building new conversion technologies is defined as follows:

$$\mathscr{I}^{\mathrm{P}}_{iy} = \varsigma \sum_{pz} D^{\mathrm{C}}_{piy} C^{\mathrm{P}}_{piy} N I^{\mathrm{PC}}_{pzy} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{4.13}$$

where C^{P}_{piy} is the technology capital impact; D^{C}_{piy} is a factor that discounts the capital cost back to start of the time horizon, taking account of how the capital is financed (for non-financial impacts, this factor is 1); and ς is a linear scaling factor to improve optimisation performance. The total net present O&M impact for conversion technologies is defined as follows:

$$\mathscr{I}^{\mathrm{fp}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} \sum_{pz} \phi^{\mathrm{P}}_{piy} N^{\mathrm{PC}}_{pzy} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{4.14}$$

where ϕ^{P}_{piy} is the technology fixed operating impact and D^{OM}_{iy} is a factor that discounts financial impacts, assumed to be made annually, back to the start of the time horizon or is equal to the number of years in period y, n^{yy}_{y}, for non-financial impacts. Finally, the total net present variable operating impact of conversion technologies depends also on the operating rates of the given technology:

$$\mathscr{I}^{\mathrm{vp}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} \sum_{pzhdt} \varphi^{\mathrm{P}}_{piy} \mathscr{P}_{pzhdty} n^{\mathrm{hd}}_{h} n^{\mathrm{dw}}_{d} n^{\mathrm{wt}}_{t} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{4.15}$$

where $\varphi^{\mathrm{P}}_{piy}$ is the variable (rate-dependent) operating impact.

4.4.1.5 CO_2 utilisation and storage

Whilst many conversion technologies generate CO_2 emissions, it is only possible for CO_2 capture technologies to capture emissions from large point sources. In the VWM, large technologies that can be coupled with CO_2 capture technologies produce a resource "CO_2" for the CO_2 that they emit. The capture technologies can convert this "CO_2" resource to "Captured CO_2", which can then be stored underground (CCS) or converted by other technologies to form useful products (CCU). The technologies that produce "capturable" CO_2 are denoted "industrial emitting technologies" (IET) and the following constraints are used to account for the amounts of CO_2 emitted, captured, utilised and stored.

The total rate of production of CO_2 from all industrial emitting technologies in each zone and at every time, $\mathscr{C}^{\mathrm{IET}}_{zhdty}$, is given by:

$$\mathscr{C}^{\mathrm{IET}}_{zhdty} = \sum_{p \in \mathbb{P}^{\mathrm{IET}}} \mathscr{P}_{pzhdty} \alpha_{p,\mathrm{CO_2}} \qquad \forall z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.16}$$

Some of this generated CO_2 can be captured by the CO_2 capture technologies (if any have been built – see Section 4.4.1.4) and the rate of capture of CO_2, which has to be utilised or stored, is given by:

$$\mathscr{C}^{\mathrm{US}}_{zhdty} = - \sum_{p \in \mathbb{P}^{\mathrm{CUS}}} \mathscr{P}_{pzhdty} \alpha_{p,\mathrm{CO_2^{cap}}} \quad \forall z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.17}$$

(Recall that $\alpha_{p,\mathrm{CO_2^{cap}}}$ is negative because CO_2 is consumed by the capture technologies.)

Economic penalties for emissions and rewards for capture and utilisation or storage are represented by the unit impacts V^{IET}_{iy} and V^{CUS}_{iy}, respectively. The two following components of the objective function are then defined for the CO_2-producing technologies (IET) and for CO_2 utilisation and/or storage:

$$\mathscr{I}^{\mathrm{IET}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} V^{\mathrm{IET}}_{iy} \sum_{zhdt} \mathscr{C}^{\mathrm{IET}}_{zhdty} n^{\mathrm{hd}}_h n^{\mathrm{dw}}_d n^{\mathrm{wt}}_t \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{4.18}$$

$$\mathscr{I}^{\mathrm{CUS}}_{iy} = \varsigma D^{\mathrm{OM}}_{iy} V^{\mathrm{CUS}}_{iy} \sum_{zhdt} \mathscr{C}^{\mathrm{US}}_{zhdty} n^{\mathrm{hd}}_h n^{\mathrm{dw}}_d n^{\mathrm{wt}}_t \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \tag{4.19}$$

The values of the cost component (i = cost) of V^{IET}_{iy} and V^{CUS}_{iy} may be different to allow CO_2 emissions to be penalised at a different rate to the rewards for CO_2 utilisation or storage.

CO_2 emissions are tracked as follows. All technologies that emit CO_2, including industrial emitters, contribute to the CO_2 component of the objective function through their impacts (C^{P}_{piy} and $\varphi^{\mathrm{P}}_{piy}$ in equations 4.13 and 4.15). Any CO_2 that is then captured, which can only be done for the "IET" technologies, is offset in the objective function by the term $\mathscr{I}^{\mathrm{CUS}}_{iy}$ for $i = CO_2$, which is exactly the amount of CO_2 captured and either utilised or stored. This requires that $V^{\mathrm{CUS}}_{\mathrm{CO_2},y}$ is set to 1 and $V^{\mathrm{IET}}_{\mathrm{CO_2},y}$ must be zero.

4.4.1.6 Storage technologies

Storage technologies are modelled similarly to production technologies: conversion factors define efficiencies and energy requirements for the operation of each storage technology, with the flows of resources being determined by the product of the operating rate and the conversion factor (cf. equation 4.9). However, storage technologies can either store excess resources, $\mathscr{S}^{\text{put}}_{szhdty}$, or retrieve them from storage, $\mathscr{S}^{\text{get}}_{szhdty}$. Thus, the equivalent of equation 4.9 for storage is:

$$S_{rzhdty} = \sum_{s} \left(\mathscr{S}^{\text{put}}_{szhdty} \sigma^{\text{put}}_{sr,\text{src},y} + \mathscr{S}^{\text{hold}}_{szhdty} \sigma^{\text{hold}}_{sr,\text{dst},y} + \mathscr{S}^{\text{get}}_{szhdty} \sigma^{\text{get}}_{sr,\text{dst},y} \right)$$
$$\forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.20}$$

where there is also an operating rate equivalent to the amount of resource in storage, $\mathscr{S}^{\text{hold}}_{szhdty}$, which allows the modelling of energy requirements for holding inventory (e.g. recondensing boiled-off natural gas in LNG storage) and losses (e.g. batteries losing charge over time). S_{rzhdty} is the net production of resource in a zone due to the operation of all storage technologies. For the resource being stored, it is negative if storage is being filled (the zone has to produce resource in order to store it) or it is positive if storage is being emptied (the zone gains resource to use by taking it out of storage). Other resources can be produced in or required of the zone, such as emissions and energy required to power the storage activities. Constraints equivalent to equations 4.10 and 4.11 restrict the rates of operation of the storage technologies, $\mathscr{S}^{\text{put}}_{szhdty}$, $\mathscr{S}^{\text{hold}}_{szhdty}$ and $\mathscr{S}^{\text{get}}_{szhdty}$, as well as tracking the numbers of storage technologies in each zone, N^{S}_{szy}.

In addition to the above constraints, the overall inventory of a given storage technology s is also calculated:

$$I_{szhdty} = n^{\text{hd}}_{h} \sum_{r} \left(\mathscr{S}^{\text{put}}_{szhdty} \sigma^{\text{put}}_{sr,\text{dst},y} + \mathscr{S}^{\text{hold}}_{szhdty} \sigma^{\text{hold}}_{sr,\text{src},y} + \mathscr{S}^{\text{get}}_{szhdty} \sigma^{\text{get}}_{sr,\text{src},y} \right)$$
$$\forall s \in \mathbb{S},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.21}$$

and constrained to ensure that it remains within the maximum storage capacity of the technologies at all times, and also to ensure that an (optional) minimum level of storage is maintained for resilience. The full set of constraints are too numerous to show here but are all given in the supplementary material[‡].

The rate at which the storage technology holds resource in storage, $\mathscr{S}^{\text{hold}}_{szhdty}$, is given by the inventory level at the end of the previous hourly interval:

$$\mathscr{S}^{\text{hold}}_{szhdty} = I_{sz,h-1,dty}/n^{\text{hd}}_{h} \quad \forall s \in \mathbb{S},\, z \in \mathbb{Z},\, h > 1 \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{4.22}$$

and $\sigma^{\text{hold}}_{sr,\text{src},y}$ is 1 minus the fraction of storage inventory lost in one hourly interval.

The impacts included in the objective function for the capital ($\mathscr{I}^{\text{S}}_{iy}$), fixed operating ($\mathscr{I}^{\text{fs}}_{iy}$) and variable operating ($\mathscr{I}^{\text{vs}}_{iy}$) impacts of storage technologies are defined in a similar way to the conversion technology impacts (equations 4.13 - 4.15).

4.4.1.7 Transport technologies

Transport of resources between zones is effected by transport technologies, which operate on transport infrastructures (e.g. trailer transport on roads, barges on inland waterways, power flows on electricity transmission lines of various types, etc.). The number and capacity of infrastructures in place between two zones limits the maximum rate of operation of each transport technology and further infrastructures can be invested in if required. Resource flows are calculated from the operating rate, $\mathscr{Q}_{mzz'hdty}$, of transport technology, l, and both distance-independent and distance-dependent conversion factors ($\bar{\tau}_{mrfy}$ and $\hat{\tau}_{mrfy}$, respectively – f = src or dst for the source or destination zone of the transport), which account for transmission losses and energy requirements for the transport (e.g. compression/pumping stations for fluid flows in pipes). Examples of how these are used to represent typical transport processes are given in the supplementary material, along with the full mathematical formulation. The net flow of resource into a zone due to the operation of transport technologies is:

[‡]The article supplementary material is not included in this thesis, but can be found with the original article.

$$Q_{rzhdty} = \sum_{z'|\nu_{z'z}=1} \sum_{l \in \mathbb{M}} \left[\left(\bar{\tau}_{lr,\text{dst},y} + \hat{\tau}_{lr,\text{dst},y} d_{z'z} \right) \mathscr{Q}_{lz'zhdty} \right] + \sum_{z'|\nu_{zz'}=1} \sum_{l \in \mathbb{M}} \left[\left(\bar{\tau}_{lr,\text{src},y} + \hat{\tau}_{lr,\text{src},y} d_{zz'} \right) \mathscr{Q}_{lzz'hdty} \right]$$
$$\forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \quad (4.23)$$

where $\mathbb{M}$ is the set of all transport processes, $\nu_{zz'}$ is a binary parameter equal to 1 if a transport connection is allowed from zone z to zone z', $d_{zz'}$ is the distance between zones z and z', and the remaining symbols have been defined previously. The first term on the right-hand side accounts for transport into the zone, from all other zones, and the second term accounts for transport out of the zone. As with production and storage technologies, the conversion factors are signed quantities: for the resource being transported, they are negative for the source zone and positive for the destination zone; otherwise they are negative when they represent resource requirements to power the transport and positive if they represent emissions.

The number of transport infrastructures between each pair of zones in each planning interval is tracked, similar to conversion technologies (equation 4.11) and storage technologies. Impacts are included in the objective function for the capital ($\mathscr{I}^{\text{Q}}_{iy}$), fixed operating ($\mathscr{I}^{\text{fq}}_{iy}$) and variable operating ($\mathscr{I}^{\text{vq}}_{iy}$) impacts of transport technologies and are defined in a similar way to the conversion technology impacts (equations 4.13 - 4.15).

4.4.1.8 Demand satisfaction

For some resources (e.g. heat and electricity), it is compulsory that demands are satisfied, so these are included in D^{comp}_{rzhdty}. For others, a demand may exist that can be optionally satisfied, receiving a revenue for doing so (e.g. CCU products); the total level of optional demand (i.e. market size) is defined by D^{opt}_{rzhdty}. The level of optional demand that is actually satisfied is the variable D^{sat}_{rzhdty}, which appears in the resource balance (equation 4.2) along with D^{comp}_{rzhdty}, and must be less than or equal to the optional demand:

$$D^{\text{sat}}_{rzhdty} \leq D^{\text{opt}}_{rzhdty} \qquad \forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \quad (4.24)$$

Revenues from the sales of resources are included in the objective function using the following impact:

$$\mathscr{I}_{iy}^{\mathrm{Rev}} = \varsigma D_{iy}^{\mathrm{OM}} \sum_{rzhdt} V_{riy} \left(D_{rzhdty}^{\mathrm{comp}} + D_{rzhdty}^{\mathrm{sat}} \right) n_h^{\mathrm{hd}} n_d^{\mathrm{dw}} n_t^{\mathrm{wt}} \qquad \forall i \in \mathbb{I},\, y \in \mathbb{Y} \qquad (4.25)$$

The parameter V_{riy} specifies the unit impact of the demand satisfaction (i.e. market price at which the resource is sold).

4.4.2 Model input data

In this study, 16 spatial zones, following the National Grid Seven Year Statement zones [68], were used to represent Great Britain. A 40-year time horizon, from 2017 to 2056, was modelled with four planning periods (decades); two season types to represent variabilities between the summer months (March – November) and the winter months (December – February); and four periods per day for modelling hourly variability.

Input data for the resources were acquired from various sources. Spatial heat and electricity data were acquired from Loughborough University data [69], and aggregated into the 16 spatial zones. The time profiles for heat and electricity demand were taken from Sansom [70] and the Gridwatch website [71] respectively, and then processed into the model time resolution. Wind speed data were obtained from the Renewables Ninja database [72, 73] and aggregated in space and time. Availabilities of natural gas production and imports were based on National Grid data [66]. For the scenarios that included availability of CO_2 from large industrial installations, this data was acquired from UK government data [74].

Input data for the properties of the conversion, storage and transport technologies shown in Figure 4-2 were also obtained from a variety of sources (all values and references are provided in the supplementary material)[§]. These include: capital investment impacts; fixed and variable operating impacts; minimum and maximum rates of operation; maximum storage capacity, injectability and withdrawal rate; and conversion factors that represent the efficiencies of the technologies as well as resource requirements and losses for storage and transport technologies.

[§]The article supplementary material is not included in this thesis, but can be found with the original article.

4.4.3 Implementation

The model was implemented in AIMMS (Advanced Interactive Multidimensional Modeling System) and solved using the CPLEX solver. A typical optimisation problem (or "scenario") consists of around 104,000 variables and around 163,000 constraints, taking about 2 hours to solve on a workstation with an Intel Xeon processor with 10 cores and 128 GB RAM. The problems are solved to an optimality tolerance of 5%, which ensures a good solution is obtained in a reasonable time.

4.5 Optimisation scenarios

A total of 135 scenarios are optimised to explore the potential contribution of CO_2 and hydrogen value chains to an energy system requiring decarbonisation and flexibility. The VWM was applied to the Great Britain (GB) energy system, as an example of a medium-sized, largely fossil-based energy system. The optimisation objective was to achieve the maximum overall net present value (NPV) for the system. Revenues can be obtained from the provision of useful services (heat and electricity), and the sale of products (e.g. methanol and liquid fuels). In all scenarios that were studied, the decarbonisation of the power and heating sectors was represented by a constraint on CO_2 emissions in the final decade. A level equivalent to a 90% reduction in emissions by 2050 compared to 1990 was chosen: whilst the UK Climate Change Act prescribes that national emissions should be reduced by 80% over this period [75], it is accepted that emissions from the power and heating sectors will require greater reductions in order to account for other harder-to-decarbonise sectors, such as the aviation sector [76]. Furthermore, emissions will need to be cut further still in order to meet the requirements of the Paris Agreement (net zero emissions by 2100) [77, 78]. Other than natural gas imports, energy imports and exports (e.g. via electricity interconnectors) are not included in this work. In real energy systems, this interconnectivity can provide additional system flexibility.

Beyond the decarbonisation constraint, various scenarios were studied with additional policies and incentives to assess their influence on the energy system. These scenarios are summarised in Table 4.1, and detailed in sections 4.5.1 - 4.5.4. Additionally, a factorial analysis was performed to assess the effects of data uncertainties, and is described in section 4.5.5.

Table 4.1: Details and key input data for the scenarios modelled and optimised

Scenario category	No. of runs in category	Constraint Payment (£/MWh)	Multiplying factor applied to storage costs	CO_2 trading price (£/tCO_2)	Methanol price (£/MWh)	Industrial CO_2 Included
Baseline	1	0	1	23	52	No
Flexibility	8	70	1 – 100	23	52	No
Economics	56	0	1	23 – 130	52 – 102	No
Industrial CO_2	6	0	1	23 – 130	52	Yes

4.5.1 Baseline scenario

The baseline scenario was used to assess the GB energy system under present day policies and with median cost estimates for technologies.

A CO_2 trading price of £23/tCO_2 was included, equal to the average UK carbon price in 2017 (UK carbon support price of £18/tCO_2 [79] + average EU ETS price of £5/tCO_2 [80]). CO_2 "trading" was modelled to represent the European Union Emissions Trading Scheme (ETS) [81], penalising large emitters of CO_2 (e.g. CCGTs) by the trading price (a "cost" to the system). To further incentivise CCUS, CO_2 utilisation and storage plants are also rewarded at the same rate for the CO_2 they sequester (a "revenue" to the system). This goes beyond the existing EU ETS policy but is a useful tool for incentivising CCUS in the model: the significance of this incentive was explored through sensitivities on the CO_2 trading price.

Market prices for the CCU products were assigned based on present day prices. A price of £52 /MWh for methanol was used, based on the 2017 average (Methanex) market price [82]. Similarly, Fischer-Tropsch fuels could be sold at £55 /bbl, estimated from [83].

4.5.2 Flexibility

An area of interest for CCUS and hydrogen based technologies is their potential for providing energy system flexibility. The response of these technologies to different flexibility-based scenarios was assessed using two main inputs: the costs of hydrogen storage, and the cost of curtailed wind power. Hydrogen storage costs were increased by factors of up to 100, representing the wide range of cost estimates found in the literature [84, 85, 86] (the effects of hydrogen storage cost assumptions were also explored in the factorial analysis: see section 4.5.5). Additionally, penalties of up to £70 per MWh were applied for any unused wind power generation, representative of the average payment made by the UK grid operator in 2017 for unused wind power [87, 88].

4.5.3 Economics

As was discussed in section 4.3, the economic characteristics of CCUS technologies are complex. Two of the main drivers for the uptake of CCUS are the CO_2 trading price, and the market price available for the sale of CCU products. Therefore, a full range of scenarios was studied in which both the CO_2 trading price and the price of methanol were varied. Fifty-six scenarios were optimised with different combinations of CO_2 trading prices ranging between £23/tCO_2 and £130/tCO_2, and methanol prices ranging between £52/MWh and £102/MWh. Although there is significant uncertainty in the long term value of the CO_2 trading price, the UK government has indicated that the price could reach £70/tCO_2 by 2030 and £200/tCO_2 by 2050 [89, 90].

4.5.4 Industrial CO_2

This study focuses on the decarbonisation of domestic heat and electricity. However, industry is another major source of greenhouse gas emissions: in 2016, 32 MtCO_2 (equivalent) were attributed to large industrial installations in the UK, with further indirect emissions from the energy supplied to industry. Evidently, this could be a significant CO_2 feedstock for CCUS processes. Therefore, in the "industrial CO_2" scenarios, these emissions from large industrial installations were made available for capture and utilisation or storage. Although this would not count towards the decarbonisation constraints imposed on the domestic sector, the revenue from the CO_2 trading price was included in the objective function, and a range of trading prices were assessed with the industrial CO_2 feedstock in place.

4.5.5 Factorial analysis

Finally, a factorial analysis was performed to assess the effects of data uncertainty on the model results. A half-factorial (2^{k-1}) analysis was carried out, using seven factors, resulting in 64 optimisation runs. The analysis was carried out using Design-Expert version 11, published by Stat-Ease, Inc. [91]. The seven uncertain factors are: CO_2 capture cost, CO_2 utilisation cost, CO_2 storage cost, electrolyser cost, hydrogen storage cost, wind turbine cost, and average wind speed.

Six of the seven factors used in the analysis included multiple input parameters, for example CAPEX and OPEX costs, and technologies of all sizes. Sensitivity ranges were estimated from the literature for each factor, and applied to all input parameters in a given factor to calculate the "low" and "high" values in the factorial analysis. Details on the factors, sensitivity ranges (including references for the estimates), input parameters and final values used in the factorial analysis are provided in Appendix C[¶].

A large sensitivity range was used for hydrogen storage costs, reflecting the wide range of data in the literature. This range is partly explained by different assumptions regarding the availability and usability of underground storage. The wind speed factor was included to reflect uncertainty in the availability of wind resource. All modelled wind speeds were scaled up/down by 20%.

4.6 Results and discussion

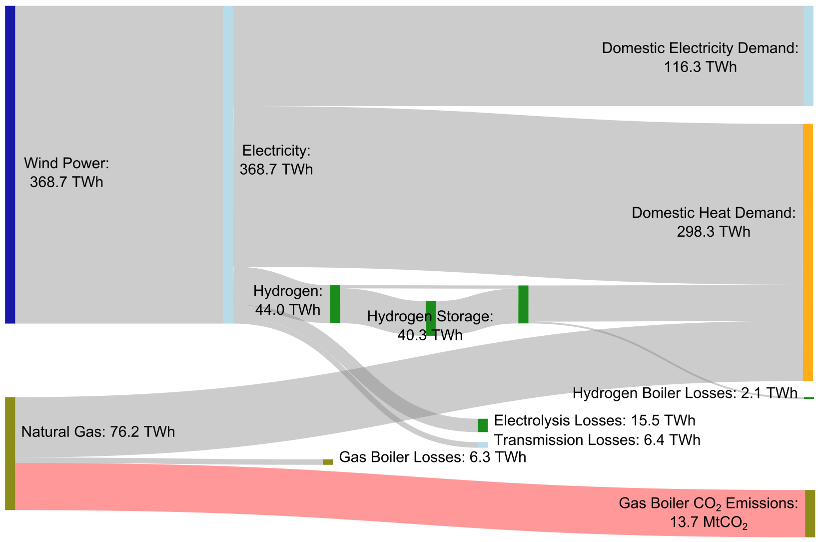
In the following sections, the results from the scenarios outlined in Section 4.5 are presented and their implications are discussed.

4.6.1 Renewables and hydrogen storage provide decarbonisation and flexibility

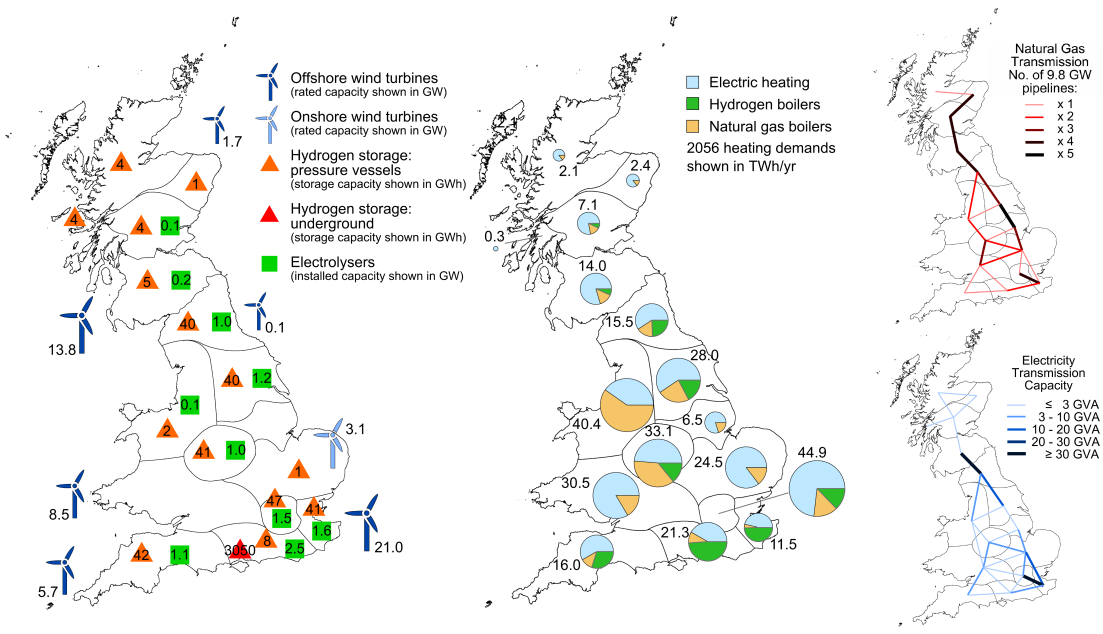
In the optimisation scenario with baseline policies, a transition occurs from the present day to a low-carbon, flexible energy system in 2056. However, no CCUS technologies are installed: decarbonisation and flexibility are provided at lower cost through renewables and hydrogen storage.

Figure 4-3 shows results for the optimal system design in 2056: 4-3a shows overall flows of energy and CO_2 and 4-3b shows maps of the system design. By 2056, all electricity generation is provided by wind turbines: all of the present day gas-fired power stations are retired over the four decades, and not replaced. The overall electricity generation base is significantly increased (by a factor of 1.6), to account for growth in electricity demand and electrification of heat. Figure 4-3a shows how domestic heating is satisfied in 2056: overall, 63% of heating demand is satisfied using electricity, and 23% using natural gas, with the remainder satisfied using hydrogen. Figure 4-3b shows the detail of how this heat is delivered in the 16 spatial zones that were modelled. As Figure 4-3a shows, all remaining CO_2 emissions in 2056 are from natural gas boilers in homes:

[¶]The original article appendices are not reproduced in this thesis, but the factorial input details are provided in Table 4.2 at the end of the article.



(a)



(b)

Figure 4-3: **Optimal energy system in the baseline scenario.** (a) Sankey diagram showing annual flows of energy (in TWh/yr) and CO_2 (in t/yr) in 2056. (b) Maps showing the optimal system configuration in 2056, including: installed capacities of key technologies (left); zonal heating demands and delivery method in 2056 (numbers give total annual demand in TWh/yr) (centre); and natural gas and electricity transmission networks (right). No other transmission infrastructures (i.e. hydrogen or CO_2 pipelines) were installed in this design.

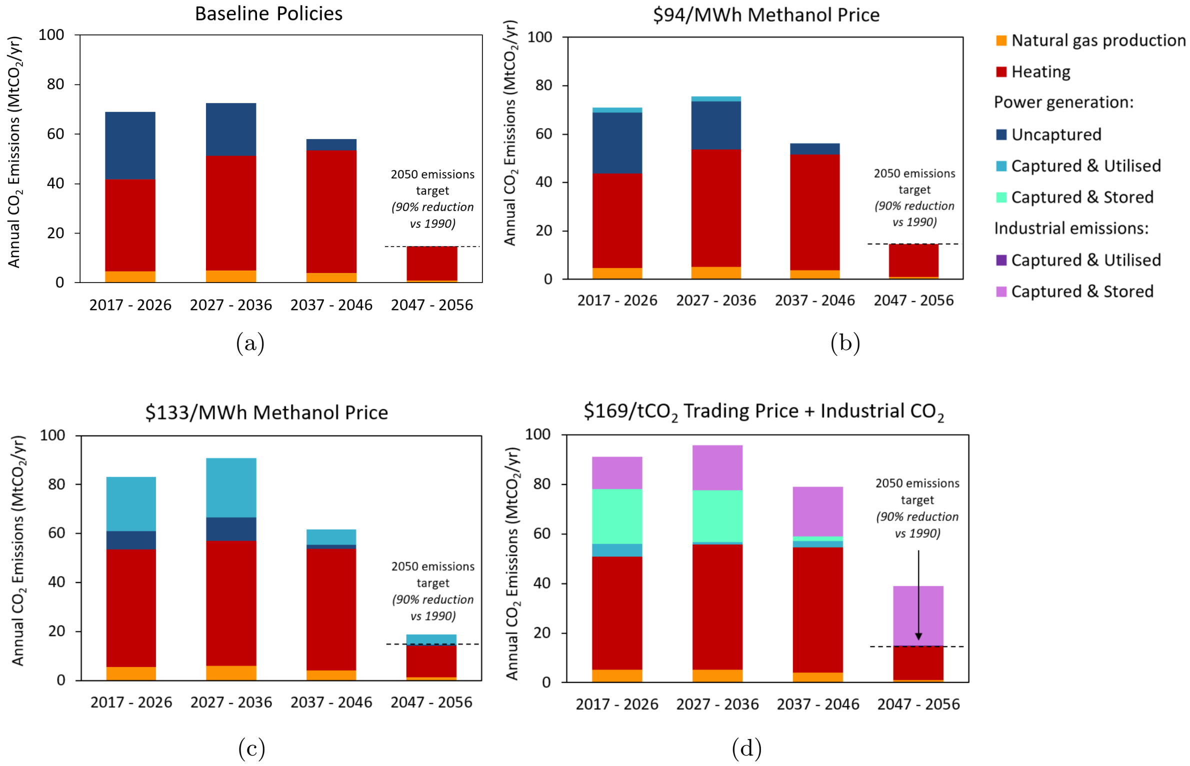


Figure 4-4: **Annual CO_2 emissions by source for four featured scenarios.** (a) Baseline policies, (b) CCU methanol price of £72/MWh, (c) CCU methanol price of £102/MWh, (d) CO_2 trading price of £130/tCO_2 and emissions from industry available for capture (but not included in emissions reduction target). For all scenarios, both captured and uncaptured emissions from power generation are shown: only uncaptured emissions are included in the net emissions level.

complete decarbonisation of power generation and significant decarbonisation of heat is sufficient to achieve the emissions reduction target in the final decade. The annual CO_2 emissions for each of the four decades modelled are shown in Figure 4-4a.

The optimal system is highly reliant on intermittent wind power but system flexibility is provided by power-to-gas and hydrogen storage. The installed capacities of these technologies in 2056 are shown in Figure 4-3b. Electrolysers are installed in many locations across the country, with a total installed capacity exceeding 10 GW. Despite SMR facilities for hydrogen production being available to build, the optimal solution only includes hydrogen production from electrolysis. Hydrogen storage facilities are also installed: most significantly, a 3 TWh underground storage at Humbly Grove in southern England. Excess wind power generation is converted to hydrogen and either immediately distributed to homes for heating or stored to be used later. The amount of hydrogen in the Humbly Grove underground storage over the course of 2056 is shown

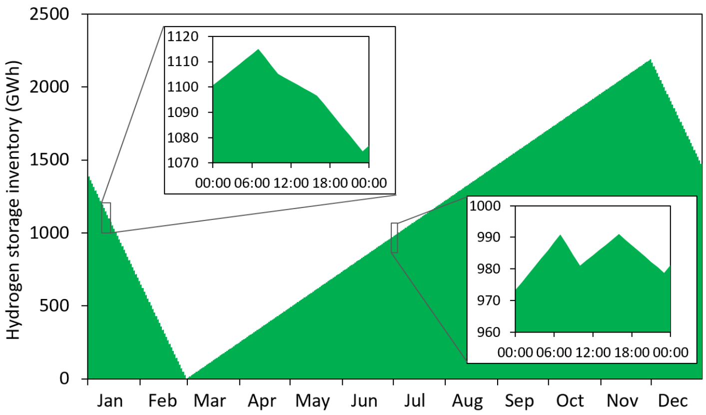


Figure 4-5: **Storage inventory for the Humbly Grove underground hydrogen storage facility throughout 2056 in the baseline scenario.** Insets show the inventory over a day in January and a day in July.

in Figure 4-5, clearly showing both inter-seasonal storage and hourly balancing.

Under these baseline assumptions, CCUS is found to be less cost effective for providing system flexibility than energy storage. In order to investigate whether CCUS could have a flexibility-providing role in the energy system, a number of additional scenarios were modelled, focusing on increasing the costs of hydrogen storage (the main flexibility provider in the baseline scenario), and the cost of curtailed wind power.

Whilst these scenarios resulted in reduced levels of curtailment and storage, the results did not include any CCUS technologies operating in a flexibility-providing role (e.g. in conjunction with dispatchable CCGT plants). It is possible that due to the high capital costs associated with CCUS, high load factors are required to justify the initial expenditure, which is not suited to operating in conjunction with "peaking" fossil fuel power plants or, in the case of CCU, only utilising hydrogen produced from excess electricity.

4.6.2 Economic incentives for CCUS

Given that under baseline assumptions, decarbonisation and flexibility constraints alone are insufficient to introduce CCUS technologies into the optimal system design, the economics of the technologies must also be explored. Primarily, this was done by varying two factors: the CO_2 trading price and the retail price of methanol. Additionally, a factorial analysis was performed, exploring the effects of different technology cost assumptions.

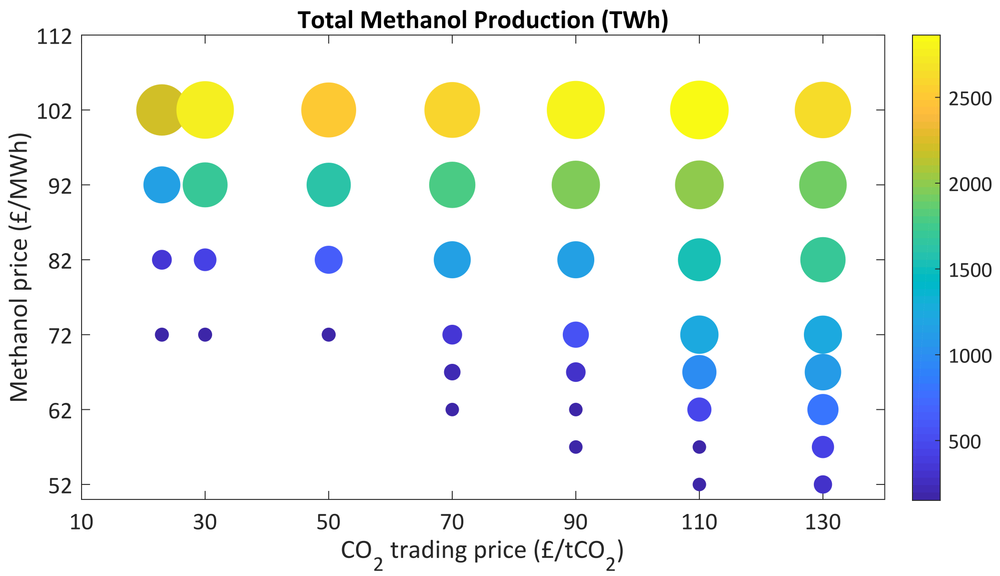


Figure 4-6: **Total methanol production (CO_2 hydrogenation) between 2017 and 2056, for a range of cases.** 56 scenarios were optimised, each with a unique combination of methanol price and CO_2 trading price. Total methanol production is represented by both the datapoint size and colour.

Figure 4-6 shows the total methanol production from CCU over the forty-year time horizon for each of the 56 scenarios that were assessed with different CO_2 trading prices and methanol prices.

Whilst a methanol market price of £52/MWh together with a CO_2 trading price of £23/tCO_2 were insufficient to incentivise methanol production from CCU, with a 40% increase in the methanol price (to £72/MWh) CCU becomes part of the optimal energy system. In this case, CO_2 capture facilities are installed at some existing CCGT plants, and the captured CO_2 is used with hydrogen from electrolysis to produce methanol in a single CO_2 hydrogenation plant. This plant produces 8.2 TWh per year, but as Figure 4-4b shows, the contribution of CO_2 utilisation to overall emissions reaches a maximum of only 2.1 MtCO_2 per year. The CCU plant operates only in the first two decades. In the later decades, as the existing CCGTs retire, they are replaced with wind power, rather than investing in new CCGTs with CCU. Consequently, by the final decade decarbonisation is achieved through renewables and heat decarbonisation. Although it may be optimal to the wider system to install and operate capital intensive CCU technologies for only two decades, in reality this strategy may be unattractive to potential investors.

With a 100% increase in the methanol price (to £102/MWh), CCU has a greater

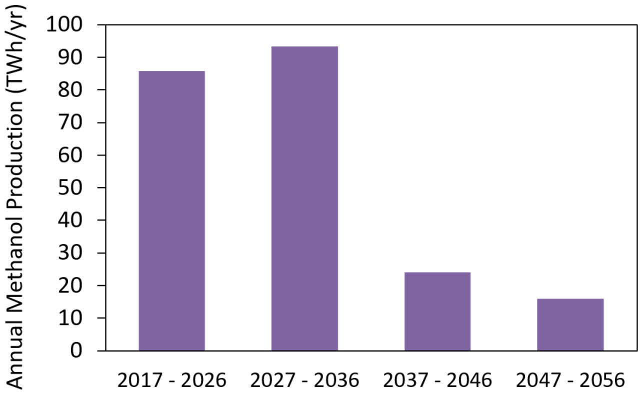


Figure 4-7: **Annual methanol production in each decade for the scenario with a methanol price of £102/MWh.**

contribution, and CCU (along with new CCGTs) is sustained throughout all decades. Figure 4-4c shows the annual CO_2 emissions for this scenario and Figure 4-7 shows methanol production rates for each of the four decades. Although CCU is operated throughout all four decades, it still has its peak in the second decade, with some CCU plants retiring when existing CCGTs retire. However, in this scenario, it is now worthwhile in some locations to invest in new CCGTs with CCU, and consequently CCU has a significant contribution to the final decade emissions target (although it should be remembered that the emissions sequestered into the CCU products will be re-emitted when the product is consumed). Figure 4-8 shows the installed capacities of key technologies (including CCU) in 2056 in this scenario. A large capacity of hydrogen storage is required to match hydrogen supplies to the demands from both CO_2 hydrogenation and domestic heating.

The level of methanol production in the final decade of this scenario is 16 TWh/yr, compared with 93 TWh/yr produced in the second decade. The market size for methanol in Western Europe is currently around 40 TWh/yr [92], therefore it is likely that new demands for methanol would need to be found, such as displacement of existing fuels. For example, demand for petroleum for road transport in the UK in 2017 was 470 TWh [93], so this could provide a market for methanol. Furthermore, whilst methanol production is the key CCU pathway in this study, in reality a more diverse selection of CCU pathways exists, producing alternative products. A methanol price of £102/MWh is considerably higher than the current market price, so would be likely to require policy support. Petroleum has a retail price in excess of £130/MWh in the UK [94], so a methanol price of £102/MWh would be competitive, however this does not

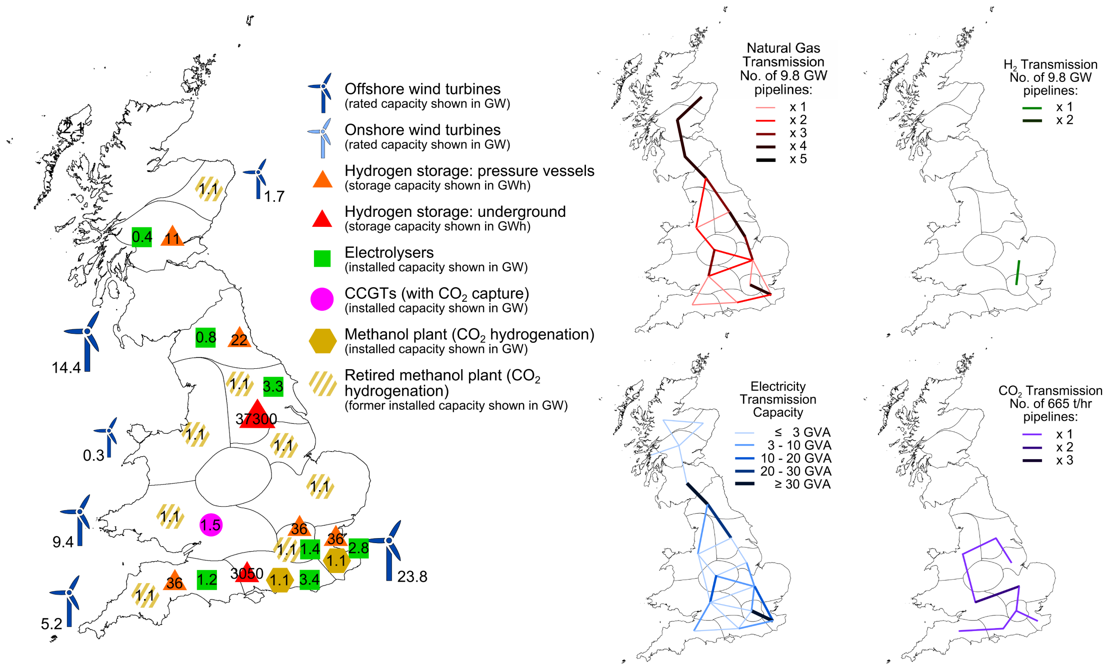


Figure 4-8: **Optimal energy system for the scenario with a methanol price of £102/MWh.** Maps show the system in 2056, including: installed capacities of key technologies (left); and natural gas, H_2, electricity and CO_2 transmission networks (right). Retired CCU plants are also displayed, indicating the scale of CCU during the early decades. In the final decade, 73% of heat demands are satisfied by electricity, 19% by natural gas and 9% by hydrogen. The hydrogen transmission pipeline in the east of England serves demands for hydrogen for heating in this region.

account for the significant levels of taxation applied to petroleum, and the subsequent loss in tax revenue.

CO_2 trading prices have some influence on the uptake of CCU for cases with a lower overall CCU uptake, but in cases with higher overall CCU uptake the influence is limited, as Figure 4-6 shows. The CO_2 trading price provides a strong incentive for CCUS in the early decades, when a large capacity of CCGTs producing by-product CO_2 still exists. These plants will be penalised by a CO_2 trading price, and only CCUS can reverse this penalty. In the later decades, once existing CCGTs have retired, the CO_2 trading price does not provide any incentive for installing CCGTs with CCUS over other types of low-carbon power generation (i.e. wind power). Hence, the CO_2 trading price has limited potential for incentivising large uptake of CCU, as this requires installation of new CCGTs with CCU once existing capacity has retired.

The limited incentive from the CO_2 trading price is also why CCS facilities, which lack an additional revenue stream, are not installed. Only with a CO_2 trading price of £130/tCO_2 does CCS become part of the optimal solution because, at this level, the costs of unabated emissions from the existing CCGTs are so high that building CCS for just the early decades is justified. This shows the importance of appropriate policies, if potentially valuable technologies such as CCUS are to be incentivised.

4.6.3 Factorial analysis

To assess the reliability of the baseline technology cost assumptions, a factorial analysis was performed consisting of 64 different optimisation scenarios. Half-normal plots of effects for four responses in the factorial analysis are shown in Figure 4-9. Selected results from all factorial analysis runs are provided in the supplementary material[‖].

The results of the factorial analysis broadly support the robustness of the baseline data assumptions. For example, the contribution of CCUS to the optimal energy system remains limited, even in the scenarios with data sensitivities most favourable to CCUS (e.g. low CCUS costs, high hydrogen storage costs). CCS facilities continue to remain absent from all scenarios. The results show an increased uptake of CCU in the scenarios most favourable to CCU. However, this is predominantly only in the early decades, meaning that the final energy system design remains largely unchanged. A possible cause for this is the significant amount of supporting infrastructure that is required for CCUS: even with optimistic assumptions regarding the costs of CCUS itself, there are still the costs of the CCGTs, CO_2 transport and, in the case of CCU, hydrogen

[‖] The supplementary material is not included in this thesis but can be found with the original article

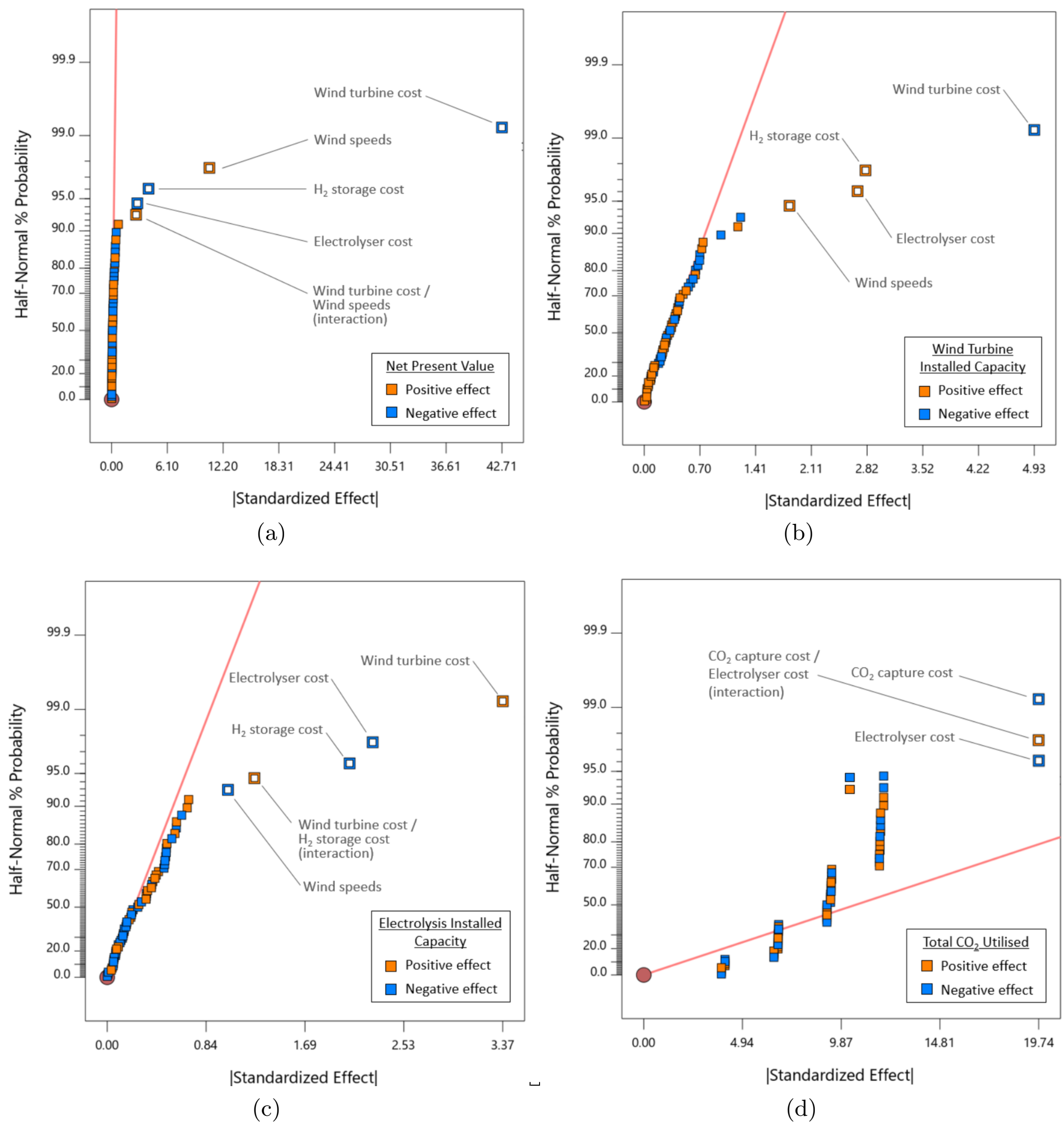


Figure 4-9: **Half-normal probability plots of effects for four responses in the factorial analysis.** (a) Net present value, (b) Installed capacity of wind turbines in 2056, (c) Installed capacity of electrolysers in 2056, (d) Total quantity of CO_2 emissions utilised over the time horizon. For each plot, the factors (and interactions between factors) with the most significant effects on the response appear further to the right, and are indicated. Orange denotes that the factor has a positive effect on the response, blue denotes negative.

supply infrastructure. Figure 4-9d shows that the costs of CO_2 capture facilities and electrolysers were the dominant factors in the uptake of CCU, more than the cost of the CO_2 utilisation plant itself. This shows that CO_2 utilisation is quite reliant on its supply chain.

Overall, wind turbine data is the most influential on the optimisation results. Wind turbine cost is the factor with the greatest effect for many model responses, including net present value. The wind speed factor also has significant effect on several responses. The importance of wind turbine data is unsurprising given the strong role that wind turbines have in the majority of optimal networks. Confidence in data assumptions for wind turbines is relatively high, as the technology is well established. In fact, given that the baseline assumptions are based on present day technologies, it is possible that improvements in cost and performance will be achieved, increasing the case for wind turbines in the optimal system design.

The factorial analysis also revealed strong interdependence between wind turbines, electrolysers, and hydrogen storage. The costs for each of these technologies are all significant factors in the final installed capacities. For example in Figure 4-9c, it can be seen that the installed capacity of electrolysers in the final system design is most dependent on wind turbine costs, followed by electrolyser costs and hydrogen storage costs. This shows the reliance that each of these technologies has on the other stages of the value chain, and the importance of the costs of all of the technologies. Despite there being a significant level of uncertainty associated with hydrogen storage costs, they are found to have a relatively small effect on power-to-gas uptake, as shown in Figure 4-9c. This is due to the small contribution that storage costs have to the overall hydrogen supply chain.

4.6.4 Emissions from industry as an additional CO_2 feedstock

As CCGT plants are retired and replaced with renewable generation in the later decades, there becomes a lack of point source CO_2 emissions, and consequently there is limited opportunity for CCUS technologies. This is particularly challenging for CCS, which has high capital expenditure and long project times, meaning that a long term supply of CO_2 is necessary to justify investment.

To address this, additional CO_2 emissions from large industrial installations were included in the optimisation. These emissions were not included in the emissions reduction target, but could optionally be captured and utilised or stored, to obtain the revenue from the CO_2 trading price.

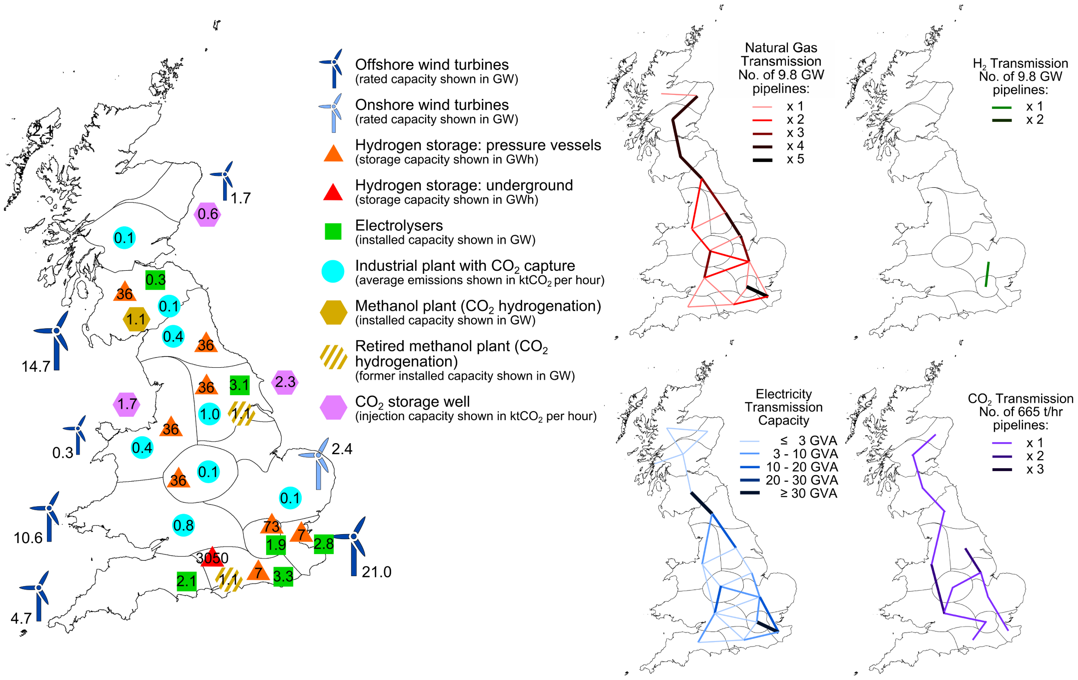


Figure 4-10: **Maps of the optimal energy system for the scenario with a CO_2 trading price of £130/tCO_2 and optional capture of CO_2 emissions from industry.** Maps show the system in 2056, including: installed capacities of key technologies (left); and natural gas, H_2, electricity and CO_2 transmission networks (right). Retired CCU plants are also displayed. In the final decade, 63% of heat demands are satisfied by electricity, 23% by natural gas and 14% by hydrogen.

Whilst these additional emissions have little effect on the uptake of CCU, they do influence CCS. With a CO_2 trading price of £130/tCO_2, CO_2 capture is installed at many locations throughout the country, and CO_2 storage wells are installed at three locations. The optimal system design in this scenario is shown in Figure 4-10. Annual CO_2 emissions for the scenario are shown in Figure 4-4d: in the early decades, CCS has a significant impact on emissions from power generation, but by 2056 power generation is again focused on wind power, and CCS is focused on emissions from industry.

4.7 Conclusions

Various CO_2 and hydrogen value chains exist that may offer potential for decarbonisation and flexibility in future energy systems. By modelling these value chains as integral components of the energy system, it has been possible to assess the merits of technologies including CCS, CCU, power-to-gas and hydrogen storage.

The results show that with baseline cost and policy assumptions, there are opportunities for CCUS to decarbonise existing power generation capacity. However, long-term decarbonisation can be achieved at lower cost through expansion of renewables, using hydrogen storage to ensure system flexibility. The high capital costs of CCUS technologies and their associated supply chains mean that it is challenging to find flexibility-based business cases, which are likely to involve low load factors for the technologies.

CCU pathways that combine captured CO_2 with renewable hydrogen are capable of producing synthetic fuels that are competitive with existing fuels. For example, methanol from CCU could be competitive with petroleum as a transport fuel, if it had a similar retail price, but it is not currently competitive with the existing market price for methanol from fossil-based sources. Despite the economic opportunity for CCU, based on existing market sizes it is unlikely that CCU will have a significant contribution to CO_2 emissions reductions, particularly considering the secondary emissions when the fuel is used.

The methodology and results presented in this study are valuable to both policymakers and potential investors for informing which technologies are likely to be valuable in future energy systems. The results also show the necessity of implementing appropriate policies, if CCUS technologies are to be incentivised. This is particularly the case for CCS. In this study, it was found that a CO_2 trading price of £130/tCO_2 was required for CCS to become part of an optimal energy system, however there may be alternative policies that can incentivise this technology more efficiently.

Whilst this study found that the decarbonisation potential of CCUS for the power and heating sectors may be limited, it is likely that the contribution would be greater in scenarios where stringent decarbonisation targets are imposed on industry, much of which is reliant on fossil fuels. However, alternative decarbonisation options for industry should also be considered, such as efficiency savings, use of low-carbon fuels (e.g. renewable hydrogen and biofuels) and electrification.

This study assessed a national energy system over a forty year period, taking into account existing installed capacities of technologies, in order to model the rate of transition to a low-carbon system. The results showed a rapid transition to renewables and expansion of hydrogen supply chains. However, it remains to be seen whether power-to-gas can be scaled up sufficiently quickly. Alternative scenarios may see more hydrogen production from fossil fuels in the medium term; in this case, there would be a greater opportunity for CCUS technologies.

Finally, this study considered the optimal configuration for a low-carbon energy system in the 2050s. It is becoming increasingly important to look beyond this target, to possible zero-carbon energy systems. In this scenario, negative emissions technologies, such as BECCS and DACS may become more relevant, and hence there may be a greater role for CCUS in the long term.

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Article appendices

Not all of the appendices from the original Applied Energy article are reproduced here. Appendix A of the original article, the abbreviations, can be found at the beginning of this chapter. Appendix B, the model nomenclature, is not reproduced but a full model nomenclature can be found in Appendix A of the thesis. Appendix C of the original article, the values used in the factorial analysis, is provided below in Table 4.2. Finally, the supplementary material for the original article is not included in this thesis but can be found with the original publication.

Table 4.2: Details of the factors used in the factorial analysis, including baseline, lower and upper values

Factor	Name	Sensitivity range	Range ref.	Parameter	Baseline Value	Low Value	High Value
A	CO_2 capture cost (£m)	+ 10% – 50%	[53]	CO_2 Capture - CAPEX	555	278	611
				CO_2 Capture - OPEX	55.5	27.8	61.1
B	CO_2 utilisation cost (£m)	+ 30% – 30%	[61]	Hydrogenation plant - S - CAPEX	22.3	15.6	29.0
				Hydrogenation plant - M - CAPEX	89.9	62.9	117
				Hydrogenation plant - L - CAPEX	358	251	465
				Hydrogenation plant - S - OPEX	1.23	0.861	1.60
				Hydrogenation plant - M - OPEX	4.95	3.47	6.44
				Hydrogenation plant - L - OPEX	19.7	13.8	25.6
C	CO_2 storage cost (£m)	+ 50% – 50%	[56, 54]	CO_2 Well - S - CAPEX	95.3	47.7	143
				CO_2 Well - M - CAPEX	137	68.5	206
				CO_2 Well - L - CAPEX	231	116	347
				CO_2 Well - S - OPEX	6.10	3.05	9.2
				CO_2 Well - M - OPEX	6.49	3.25	9.7
				CO_2 Well - L - OPEX	7.67	3.84	11.5
D	Electrolyser cost (£m)	+ 50% – 50%	[44]	Electrolyser - S - CAPEX	8.04	4.02	12.1
				Electrolyser - M - CAPEX	20.4	10.2	30.7
				Electrolyser - L - CAPEX	31.6	15.8	47.3
				Electrolyser - S - OPEX	0.402	0.201	0.603
				Electrolyser - M - OPEX	1.02	0.511	1.53
				Electrolyser - L - OPEX	1.58	0.789	2.37
E	H_2 storage cost (£m)	+ 1000% – 90%	[84, 85, 86]	CGH2S - S - CAPEX	4.07	0.407	44.8
				CGH2S - M - CAPEX	23.5	2.35	258
				CGH2S - L - CAPEX	135	13.5	1,489
				US-H2 - Ald - CAPEX	429	42.9	4,719
				US-H2 - Hum - CAPEX	61.0	6.10	671
				US-H2 - Rou - CAPEX	280	28.0	3,080
				US-H2 - War - CAPEX	200	20.0	2,198
				CGH2S - S - OPEX	0.0815	0.00815	0.896
				CGH2S - M - OPEX	0.469	0.0469	5.16
				CGH2S - L - OPEX	2.71	0.271	29.8
				US-H2 - Ald - OPEX	8.58	0.858	94.4
				US-H2 - Hum - OPEX	1.22	0.122	13.4
				US-H2 - Rou - OPEX	5.60	0.560	61.6
				US-H2 - War - OPEX	4.00	0.400	44.0
F	Wind turbine cost (£m)	+ 30% – 30%	[95]	Turbine - Offshore - CAPEX	10.8	7.56	14.0
				Turbine - Onshore - CAPEX	2.50	1.75	3.25
				Turbine - Offshore - OPEX	0.235	0.165	0.306
				Turbine - Onshore - OPEX	0.0545	0.0382	0.0709
G	Wind availability	+ 20% – 20%	[73]	Wind Speed Factor	1	0.8	1.2

Chapter concluding remarks

The article that has been presented in this chapter contains several valuable contributions to the thesis, including the introduction and development of the modelling approach, discussion of the issues concerning hydrogen and CO_2 value chains, and pertinent results on the potential for hydrogen and CCUS in the GB energy system.

The article has introduced the primary modelling tool for the thesis, the VWM, and demonstrated some of the strengths that it has for modelling interconnected energy value chains. The article has shown that the VWM has many of the modelling characteristics that were identified in Chapters 2 and 3 as being essential for accurately representing hydrogen and related flexibility technologies. In particular, this includes technological, spatial and temporal detail, although the level of detail that can be achieved is subject to tradeoffs with computational tractability.

In this chapter, a more detailed representation of CO_2 value chains was included in the VWM. Detailed representation of CO_2 is important for any energy system model that seeks to measure environmental impact, due to the myriad sources of CO_2 emissions throughout energy value chains. This representation also enables accurate modelling of CCUS technologies.

Moreover, CO_2 value chains are intrinsic to many energy value chains, including hydrogen, so the additions made in this chapter will be valuable for modelling hydrogen in future chapters. For example, any fossil fuel based hydrogen production value chains are likely to require CCUS in order to produce sufficiently low-carbon hydrogen.

In addition to demonstrating the functionality of the VWM, the scenarios explored in this chapter provide some interesting insights into the potential for CCUS and hydrogen technologies in the GB energy system. Most significantly, the results suggest that decarbonising the GB heat and electricity sectors may be achieved most cost effectively through scale-up of renewable electricity, with a limited role for CCUS. In future chapters, more energy system details will be incorporated into the scenarios, for example also including commercial and industrial sectors, and "peak" energy demands. These additions may introduce new opportunities for CCUS.

Another interesting result from the study is that where hydrogen arises in the scenario results, it is predominantly in a sector-coupling, flexibility role, rather than as a direct energy supply chain (for example decarbonisation of heat). An example of this is shown in Figure 4-3, where it can be seen that the vast majority (92%) of all hydrogen in the system flows through storage in between production and end-use. Furthermore, the cases with methanol production via CCU are an example of sector-coupling: power-to-gas hydrogen enables the linking of the electricity sector with the industrial or transport sectors (depending on the end-use of the methanol). This finding will be explored further in the following chapters.

In Chapters 5 and 6, further modelling scenarios will be explored, including representation of peak demands and inclusion of sectors beyond the domestic sector. Furthermore, hydrogen and associated value chains will be represented in more detail, for example by including gas and electricity distribution grids, linepack (on both the gas distribution and transmission grids), and the interfacing of hydrogen with these systems (e.g. through hydrogen injection into the gas grid).

The following clarifications to the article presented in this chapter should be noted, which have been identified since the article was published:

- In Figure 4-2, the meaning of "two representative zones" is not clear. These are two representative spatial zones, for example representing regions of a country. Each spatial zone can have its own resource availabilities (e.g. wind and solar) or demands (e.g. heat or electricity). As the diagram illustrates, each of the technologies included in the model can optionally be installed in a spatial zone (subject to any constraints, e.g. land use). Additionally, transportation technologies can be installed, to move resources between spatial zones. Two representative zones are shown in Figure 4-2, but any number of zones may be modelled in practice (16 spatial zones are used to represent Great Britain in this thesis).
- It should be noted that Equation 4.4 is essentially the Betz equation.
- In Figure 4-9, the meaning of the red lines is not clear. These lines represent the smallest 50% of effects in each graph. Effects to the left of the line are the least significant, whereas the further that effects are to the right of the line, the more significant they are.
- In section 4.7, it is stated that "the methodology and results presented in this study are valuable to both policymakers and potential investors", where it should state that "the methodology and results presented in this study are *intended to be* valuable to both policymakers and potential investors"

Chapter 5

Should we inject hydrogen into gas grids? Practicalities and whole-system value chain optimisation

Chapter introductory remarks

This chapter is based on the research article published by Elsevier in Applied Energy. The publisher permits the re-use of the article in this thesis, provided that the journal is referenced as the original source. The article details are as follows:

> Christopher J. Quarton and Sheila Samsatli. Should we inject hydrogen into gas grids? Practicalities and whole-system value chain optimisation. *Applied Energy*, 275:115172, 2020. https://doi.org/10.1016/j.apenergy.2020.115172

The study presented in this chapter incorporates many of the modelling requirements for hydrogen and gas grids that were identified in Chapters 2 and 3 into the powerful energy value chain optimisation model that was introduced in Chapter 4. In particular, Chapter 2 introduced the concept of hydrogen injection into gas grids and reviewed approaches for modelling the process; Chapter 3 identified the key requirements for models to accurately represent hydrogen within energy systems; and in Chapter 4 it was shown that the Value Web Model meets many of these requirements. In this chapter, the Value Web Model is configured, and scenarios are developed, that include a more detailed representation of hydrogen injection into gas grids and the associated technologies. As a result, this chapter represents the most significant development of the modelling method in this thesis.

The study presented in this chapter starts with a deeper introduction to hydrogen injection into gas grids, considering both the advantages and practical challenges for injection. Key design and operational aspects of existing gas grids are discussed, including linepack flexibility. Finally, the implications of hydrogen injection on these existing behaviours are considered. This information is valuable for understanding the realistic potential for using hydrogen with existing natural gas infrastructures, and was also used directly to inform the modelling work.

The modelling developments carried out in this study are clearly presented within the article. The key addition in this chapter, that allows for representation of hydrogen injection into gas grids, is the inclusion of distribution networks. Firstly, this allows the costs of building and operating these networks to be represented, which is important as these costs may make a significant contribution to overall energy costs. For natural gas and hydrogen, including distribution networks also means that their linepack flexibility can be modelled, and as the article shows, linepack flexibility has an important role in present-day energy system operation. The representation of gas transmission networks is also developed in this study so that linepack flexibility on these networks can be included. Finally, the option for hydrogen to be injected into natural gas distribution grids, either partially or via complete conversion, is also included.

Further additions are made to the scenarios that are modelled in this chapter in order to provide a wider representation of the energy system. On the supply side, a notable addition was solar power, including representation of available land areas for installing solar PV and solar irradiance data for each spatial zone. On the demand side, while electricity and heat demands were previously limited to the domestic sector, data for commercial and industrial sectors were obtained for this study and included in the model. A “peak” demand season was also included to ensure that sufficient peak energy delivery capacity would be installed in optimised scenarios. The addition of these demands necessitated the inclusion of new conversion technologies, such as commercial and industrial heating technologies.

A *Data in Brief* article was compiled to accompany the study presented in this chapter, and includes all of the resource and technology data that was input into the model. The details and contents of this *Data in Brief* article can be found in Appendix B of this thesis.

As well as presenting all of these methodological developments, the study in this chapter also uses modelling scenarios to consider the role of hydrogen injection into the gas grid in the Great Britain energy system. These scenarios are intended to illustrate the functionality of the model whilst also providing insights into the outlook for partial hydrogen injection in the short term, and conversion of gas grids to hydrogen as a long term option. The implications of these insights are discussed both within the article, and in the concluding remarks to this chapter.

Following this introduction, an authorship declaration is provided, followed by the article as accepted for Applied Energy (although re-formatted for this thesis). The article includes its own reference list. The original article appendices are not presented in this chapter, but a guide to where the contents of the original appendices can be found is provided at the end of the article. Finally, some concluding remarks are provided at the end of the chapter, including further discussion of the contribution of the article, and its relevance to this thesis.

Authorship declaration

This declaration concerns the article entitled:

Should we inject hydrogen into gas grids? Practicalities and whole-system value chain optimisation

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Statement from candidate	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.

Signed		**Date**	16/11/2020

Article:

Should we inject hydrogen into gas grids? Practicalities and whole-system value chain optimisation

Abstract

Injection of hydrogen into existing natural gas grids, either partially or as a complete conversion, could decarbonise heat and take advantage of the inherent flexibility that gas grids provide in a low-carbon future. However, hydrogen injection is not straightforward due to the differing properties of the gases and the need for low-cost, low-carbon hydrogen supply chains. In this study, an up-to-date assessment of the opportunities and challenges for hydrogen injection is provided. Through value chain optimisation, the outlook for hydrogen injection is considered in the context of a national energy system with a high reliance on natural gas. The optimisation captures the operational details of hydrogen injection and gas grid flexibility, whilst also modelling the wider context, including interactions with the electricity system and delivery of energy from primary resource to end-use. It is found that energy systems are ready for partial hydrogen injection now, and that relatively low feed-in tariffs (£20-50/MWh) could incentivise it. Partial hydrogen injection could provide a stepping stone for developing a hydrogen infrastructure, but large scale decarbonisation of gas grids requires complete conversion to hydrogen. Whether this solution is preferable to electrification in the long term will depend on the value of the gas grid linepack flexibility, and the costs of expanding electricity infrastructure.

Abbreviations: BECCS: Biomass Energy Carbon Capture and Storage; CCS: Carbon Capture and Storage; CO_2: Carbon dioxide; DACCS: Direct Air Carbon Capture and Storage; FIT: Feed in Tariff; GB: Great Britain; GHG: Greenhouse Gas; H_2: Hydrogen; LTS: Local Transmission System; MILP: Mixed Integer Linear Programming; NETs: Negative Emissions Technologies; NTS: National Transmission System; SMR: Steam Methane Reforming; STP: Standard Temperature and Pressure; tCO_2: Tonnes of Carbon dioxide; VWM: Value Web Model.

5.1 Introduction

Energy use contributes 70% of greenhouse gas (GHG) emissions globally, so strategies are needed to eliminate these emissions in order to meet climate change targets [1]. While technologies are emerging that can enable low-carbon energy production, management and end-use, it is unclear how these technologies will be implemented to deliver low-carbon or even zero-carbon energy systems. Furthermore, whilst technologies such as renewable power and carbon capture and storage (CCS) make electricity decarbonisation increasingly achievable, other sectors, such as transport, industry and buildings have less obvious decarbonisation options [2].

The extensive use of natural gas worldwide is an example of this. Globally, over 36,000 TWh of natural gas was consumed in 2017, of which 39% was used for electricity, 32% in industry and 21% in buildings [3]. There are over 2.9 million km of high pressure gas transmission pipelines worldwide [4], and several million km more of pipelines in the low pressure distribution systems used to provide energy to buildings for heating and cooking. Figure 5-1 shows a map of countries where households are connected to gas distribution grids. In at least seven countries (including the USA, UK, Italy and Australia) more than 50% of households are connected to gas grids [5]. In the UK, for example, 86% of homes are connected to the gas grid [5], and 561 TWh of gas was delivered through the system in 2017, contributing approximately 22% of UK GHG emissions when combusted [6, 7].

Eliminating these emissions is not straightforward, as they are generated at end-use, by each household. The preferred option for reducing GHG emissions may be to abandon gas grids altogether and opt for electrification. However, electrification of heat would require a significant expansion of electricity infrastructure [8], as well as retro-fitting of homes to make them suitable for electric heating technologies such as heat pumps [9]. Meanwhile, gas grids are valuable assets, and maintaining them may be advantageous [10].

For these reasons, injecting hydrogen into gas grids, either through partial mixing with natural gas or as a complete conversion to hydrogen, is appealing. Hydrogen is gaining interest as a low-carbon energy carrier [11], due to its relatively high energy density, multiple production options (including from electricity, fossil fuels and bioenergy), and similarities in behaviour to conventional "fuels" such as methane (which is the principal component of natural gas) [12]. Potential applications for hydrogen include: transport fuel (particularly for long-range and heavy duty use, e.g. freight and shipping) [2]; decarbonising industry (for heating, and in processes such as refining and steel produc-

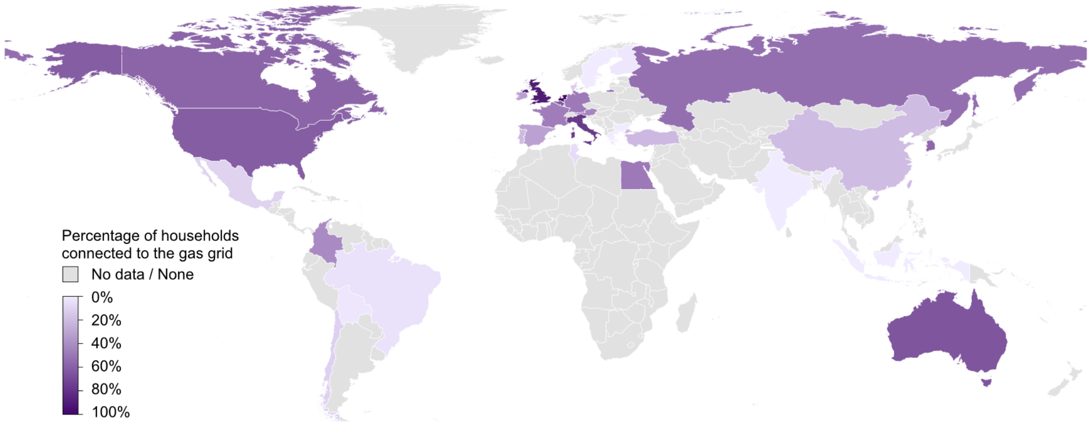


Figure 5-1: **Percentage of households connected to the gas grid in selected countries.** Data from [5].

tion) [13]; and grid-scale electricity storage [14]. Injecting hydrogen into gas grids can reduce or eliminate emissions from heating and cooking in buildings, whilst maintaining a valuable gas infrastructure (and without requiring significant upgrades to electricity infrastructure). Although end-use appliances such as cookers and boilers would need to be changed for higher levels of hydrogen injection, the overall impact on gas-heated homes would be smaller than for electrification [9].

Nonetheless, there are practical, technical and economic challenges for hydrogen injection into gas grids. Haeseldonckx & d'Haeseleer [15] and Gondal & Sahir [16] both reviewed these challenges, arguing that whilst there are clear advantages of a hydrogen-based gas system, the transition from the present system to that end-point is not obvious. There is an increasing body of evidence from projects such as NaturalHy [17] and Hy4Heat [18] that is helping to reduce the uncertainties surrounding hydrogen in gas grids. These issues are discussed in section 5.2 of this article.

Quarton & Samsatli [19] reviewed both real-life projects and modelling studies concerning hydrogen injection into the gas grid and found a growing interest in the process. Over 20 projects have injected hydrogen into gas grids or plan to do so, including several projects in Europe that produce hydrogen from electrolysis (known as power-to-gas) and inject this into the gas grid at low levels (typically up to 5 vol.%). Also of interest are recent projects aimed at understanding the practical issues of partial hydrogen injection in more detail, such as the HyDeploy project in the UK [20] and the GRHYD project in France [21]. Both of these projects are currently injecting hydrogen at up to 20 vol.% into small, private grids that deliver gas to homes and businesses. These projects are intended to validate the safety of this process and pave the way for larger projects. In the past year there has been considerable interest in hydrogen injection into the gas grid, with several new projects announced with scales of up to 100 MW, although these are still mostly at the planning stage [22].

As for modelling studies, Quarton & Samsatli [19] found that many previous studies have focussed on the business case for hydrogen injection for the hydrogen producer, such as Guandalini et al. [23], or else calculated the levelised cost of the hydrogen produced, such as Schiebahn et al. [24] and Parra et al. [25]. Some studies such as Abeysekera et al. [26] and Pellegrino et al. [27] have carried out detailed simulation of gas pipelines with hydrogen injection, providing useful insights into the behaviour of hydrogen in gas grids. However these studies have no representation of the interface with electricity and no consideration of the economics of hydrogen injection. Ogbe et al. [28] optimised natural gas pipelines with injection of hydrogen from power-to-gas, but also focussed on the details of pipeline flow rather than impacts on the wider energy system. Finally, some studies have modelled the effect of hydrogen injection on the wider energy system but these studies tend to over-simplify the process, for example lacking any spatial representation of gas grids (e.g. [29, 30]), or failing to accurately account for the differing properties of hydrogen compared to natural gas (e.g. Qadrdan and co-workers [31, 32], and Clegg and Mancarella [33, 34]).

In this paper, we start (in section 5.2) by providing an up-to-date review of the opportunities and challenges for partial injection and complete conversion of natural gas grids to hydrogen. Then (in section 5.3), we present a value chain optimisation model that represents the flows of resources from primary energy to final demand, including comprehensive representation of gas grids and hydrogen injection. We apply this optimisation model to the Great Britain (GB) energy system, as it is representative of a system with stringent decarbonisation targets and significant reliance on the gas grid. The results from this optimisation are presented in section 5.4, along with some discussion of the outlook for hydrogen injection. Finally, conclusions are provided in section 5.5.

The value chain optimisation model presented in this paper can represent all of the value chains in an energy system, from primary energy (e.g. natural gas or renewables) to end-use (e.g. electricity or heat). The costs and efficiencies of all of the processes in these value chains are accounted for, including conversion between energy carriers (e.g. gas turbines or electrolysers), generation of GHG emissions, and injection into gas grids. The model can find the overall system optimum (e.g. the system with lowest overall cost, lowest GHG emissions or other suitable metric), and can compare alternative value chains (e.g. electrification of heat vs. hydrogen injection) in their optimal configurations. This study is the first to model gas grids and hydrogen injection in energy value chain optimisation and attempts to accurately represent the details of hydrogen injection whilst also modelling the interactions with other aspects of the energy system and finding the overall system optimum.

5.2 Opportunities and challenges for using hydrogen with existing natural gas infrastructures

5.2.1 Opportunities for hydrogen injection

5.2.1.1 Power-to-gas

The term “power-to-gas” has been given various definitions; in this article, it is used to describe the process of converting electricity to hydrogen via electrolysis. Several reviews detailing the technologies and issues surrounding power-to-gas have been written, such as Schiebahn et al. [24] and Buttler & Spliethoff [35]. Arguments for power-to-gas are often based on increasing levels of intermittent renewable electricity (from wind and solar) leading to times where electricity production exceeds electricity demand. This is already happening in many countries including the UK, Germany and France, usually shown by electricity prices falling below zero [36, 37]. If hydrogen is produced from this low-cost, excess electricity, it can be used for a variety of applications, such as in transport, industry, or stored and reconverted to electricity when demands exceed supply.

Another outlet for hydrogen from power-to-gas is injection into the gas grid. Hydrogen can be directly injected into natural gas grids, either to mix with the existing natural gas, or as a complete replacement (100% hydrogen). The practical issues with each of these options are discussed in section 5.2.2. Hydrogen can also be reacted with carbon dioxide (CO_2) to form “synthetic natural gas” (i.e. methane), which can be directly injected into gas grids without any technical issues [38]. Whilst injection of synthetic natural gas shares some of the advantages of direct hydrogen injection, it does not enable the reduction of end-use GHG emissions so is not the focus of this study.

The economic case for direct hydrogen injection into gas grids is complex. Usually, natural gas is cheaper than electricity, so it is unlikely that hydrogen from power-to-gas would be cost competitive with natural gas [24]. Whether power-to-gas hydrogen can compete with natural gas in gas grids will depend on the value of absorbing excess electricity (e.g. negative electricity prices could lead to lower-cost hydrogen), and any value put on the CO_2 mitigation of hydrogen [23, 39]. Falling electrolyser capital costs will also increase the opportunities for hydrogen to compete economically with natural gas [40].

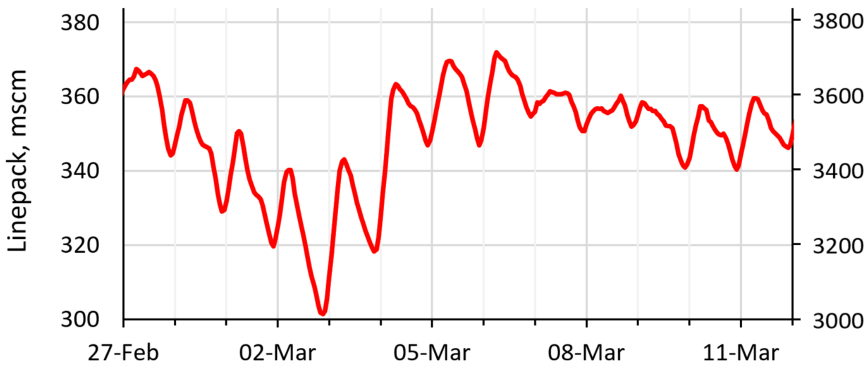
In general, the capacities of gas systems are large relative to their electricity counterparts, so gas grids could easily absorb hydrogen from excess electricity. Furthermore, gas grids have inherent gas storage capacity, known as linepack, which is described in detail in section 5.2.1.2. In fact, it is highly unlikely that power-to-gas could supply all of the gas requirements of a gas system, due to the scale of electricity production capacity that would be required. For example, in 2017, the UK gas distribution system delivered 561 TWh of gas to consumers, compared to a total national electricity production of 336 TWh (of which 62 TWh was from wind, wave or solar) [6, 41]. Consequently, it is more likely that power-to-gas would supplement other gas supplies, either supplementing natural gas in the case of hydrogen-natural gas blending, or supplementing hydrogen produced by other means, for example methane reforming (which could include CCS for a low-carbon solution).

5.2.1.2 Gas grid linepack flexibility

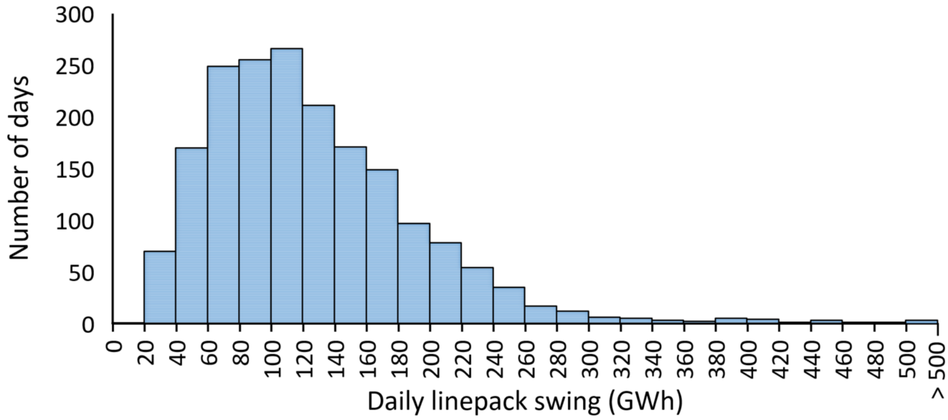
An aspect of gas grids that makes them particularly useful to energy systems is their inherent storage capacity, known as linepack [42]. The gas grid linepack is the total quantity of gas (usually measured in standard cubic metres, scm) contained within the pipelines on the network. Because the overall pressure level of these pipelines can be varied, the quantity of gas stored is also varied. High pressure gas systems, such as national and regional transmission systems, have greater linepack flexibility due to larger pressure ranges and pipeline volumes [43].

Linepack is varied throughout each day by the gas grid operators in order to balance supplies and demands of gas. As an example, Figure 5-2 shows data from the UK National Transmission System (NTS). Figure 5-2(a) shows the linepack over a ten day period in 2018, including an "extreme" demand event due to exceptionally cold weather. Figure 5-2(b) shows a histogram of linepack swing data over a 5-year period. Linepack swing refers to the difference in linepack between the beginning of the gas day (5 a.m. for the UK NTS) and the minimum level over the subsequent 24 hours [44]. Therefore linepack swing provides a measure of the overall daily flexibility of the gas grid.

On the UK NTS, daily linepack swing is commonly around 100 GWh, and in extreme events it can be more than 400 GWh. A recent study that accessed data from the UK Local Transmission System (LTS) found that the linepack flexibility offered from the LTS is of a similar size, with an average daily linepack swing of around 150 GWh, and



(a)



(b)

Figure 5-2: **Linepack data for the UK National Transmission System (NTS).** (a) Hourly linepack over a two-week period in 2018, including an extreme cold weather event; (b) Histogram of the daily linepack swing between 2013 and 2018. Data from [6].

more than 300 GWh in extreme events [43]. Linepack data for other countries is less easily available, but several countries have more extensive gas transmission systems than the UK, including the USA, the Netherlands and Japan [5], so are likely to have similar or greater linepack flexibility available.

Linepack flexibility is an essential tool for balancing supplies and demands of gas: typically, NTS linepack is depleted when gas power plants are ramped up to meet electricity peaks, whilst LTS linepack is depleted to meet increases in demand for gas for heating and cooking in homes. Therefore, if gas grid linepack were to be used for absorbing large amounts of energy from the electricity system via power-to-gas, it would be important to ensure that the existing capabilities of the system for balancing of gas supplies and demands were not reduced. This should not be a major challenge, as the scale of linepack flexibility available on the gas system is very large compared to the flexibility needs of the electricity system. For example, pumped hydro storage facilities used for within-day electricity flexibility rarely exceed 10 GWh in size [45], which is only 4% of the typical daily linepack swing on the entire UK gas grid (NTS and LTS). Furthermore, depending on the energy system dynamics, gas grid injection from power-to-gas may in fact complement the operation of the gas system, restoring gas grid linepack following a depletion.

5.2.1.3 Other opportunities

An advantage of hydrogen injection into gas grids is the reduction in GHG emissions from the gas end-use. Partial injection can achieve small GHG emissions reductions, although due to the lower energy density of hydrogen (see section 5.2.2.1), emissions reductions are relatively small: for example, hydrogen injection of 20 vol.% reduces the GHG emissions of the final gas blend by only 7%.

Complete conversion of gas grids to hydrogen would eliminate GHG emissions at end-use (and potentially the overall GHG emissions, provided the hydrogen was produced in a low-carbon manner). Therefore this option is appealing for energy systems with a heavy reliance on gas distribution systems for heating in buildings. The H21 project [46] is a proponent of this option, having designed and costed a plan for converting the gas distribution system for the north of England, and subsequently the rest of the UK, to hydrogen.

There may also be wider infrastructure benefits to injecting hydrogen into gas grids. By allowing partial, variable injection of hydrogen into gas grids, a guaranteed outlet for hydrogen is available for hydrogen producers. This can help to overcome the "chicken-and-egg" problem, whereby there is little incentive to develop hydrogen production facilities without any significant, reliable demand for the hydrogen. In this scenario, it may be necessary to provide additional economic incentives for the injected hydrogen, such as a feed-in tariff (FIT), to augment the relatively low price of gas [39]. Similarly, there may be opportunities for hydrogen injection into gas grids in conjunction with wider hydrogen projects. The HyNet project in the north-west of England, for example, proposes producing hydrogen from steam-methane reforming (SMR) with CCS, primarily for use in industry, but with the option to also feed some hydrogen into the nearby gas grids [47].

5.2.2 Challenges for hydrogen injection

Despite the opportunities for hydrogen injection, there are several practical challenges that must be overcome for hydrogen to be injected into existing natural gas infrastructures.

5.2.2.1 Pipeline energy delivery

Due to the differing thermophysical properties of hydrogen and natural gas, the pipeline energy delivery rate of the two gases also differs. This affects both complete conversion of natural gas pipelines to hydrogen and partial injection.

An expression for the energy delivery rate (i.e. the power, in MW) of gas in a pipeline is shown in equation 5.1:

$$H = u_n Q_n \tag{5.1}$$

where H is energy delivery rate; u_n is the gas energy density at Standard Temperature and Pressure (STP); and Q_n is the volumetric flow rate at STP. The volumetric flow rate can be calculated using the general flow equation for steady state gas flow (here assuming a horizontal pipe) [26]:

$$Q_n = \sqrt{\frac{\pi^2 \rho_{air}}{64}} \frac{T_n}{p_n} \sqrt{\frac{(p_1^2 - p_2^2) D^5}{fSLTZ}} \tag{5.2}$$

where ρ_{air} is the density of air at STP; T_n and p_n are the temperature and pressure at STP; p_1 and p_2 are the inlet and outlet pressures; D is the pipe diameter; f is the friction factor; S is the gas specific gravity; L is the pipe length; T is the gas temperature; and

Z is the gas compressibility factor (the volume of the real gas divided by the volume of a perfect gas at the same temperature and pressure).

Due to hydrogen's low mass density, it has a low energy density compared to natural gas (3.0 kWh/m^3 at STP, compared to around 9.9 kWh/m^3 for natural gas [41, 48]). However, as can be seen in equation 5.2, the low mass density (i.e. low specific gravity S) means that hydrogen will achieve higher volumetric flow rates than natural gas, for the same pressure drop. These factors are captured in the Wobbe number (WN), an index used in the gas industry to indicate interchangeability of gas types [49]:

$$WN = \frac{u_n}{\sqrt{S}} \tag{5.3}$$

However, there are further factors that cause differences in the flow of natural gas and hydrogen in pipelines; the most significant are the compressibility factor (Z) and kinematic viscosity (which influences friction factor f) [26]. The interaction of these factors is complex and can depend on the absolute pressure level of the pipeline and the pipe geometry. Equations 5.1 and 5.2, in combination with approximations for parameters such as the friction coefficient, can be used to estimate these effects [26, 50]. Calculations were performed to estimate the reduction in pipeline energy delivery for increasing levels of hydrogen injection, assuming a constant pipeline pressure drop. Full details of the calculations are provided in the supplementary material*, and the results are shown in Figure 5-3. The calculations assumed smooth pipe flow, which is reasonable based on the flow regime and relatively low roughness of typical gas pipeline materials. Properties for pure methane were used to represent natural gas; natural gas typically has a methane content in excess of 80 vol.% [51]. At up to around 50 vol.% injection, the behaviour is linear. Higher pressures worsen the reduced energy delivery effect of hydrogen, primarily due to the lower compressibility of hydrogen at higher pressures. For an 80 bar inlet, typical of a high pressure transmission pipeline, only around 64% of the energy can be delivered with 100% hydrogen compared with 100% methane, assuming the same pressure drop.

The lower energy density of hydrogen also means that the linepack flexibility available from a pipeline carrying hydrogen is lower than for natural gas. This effect is worsened at higher pressures by the lower compressibility of hydrogen compared to natural gas. Usable pipeline linepack swing is dependent on pipeline flow rate and the range in pressures over which the pipeline can be "swung". The effect of hydrogen injection on the available linepack flexibility of a natural gas pipeline was calculated, based on typical

*The original article supplementary material can be found in Appendix C of this thesis.

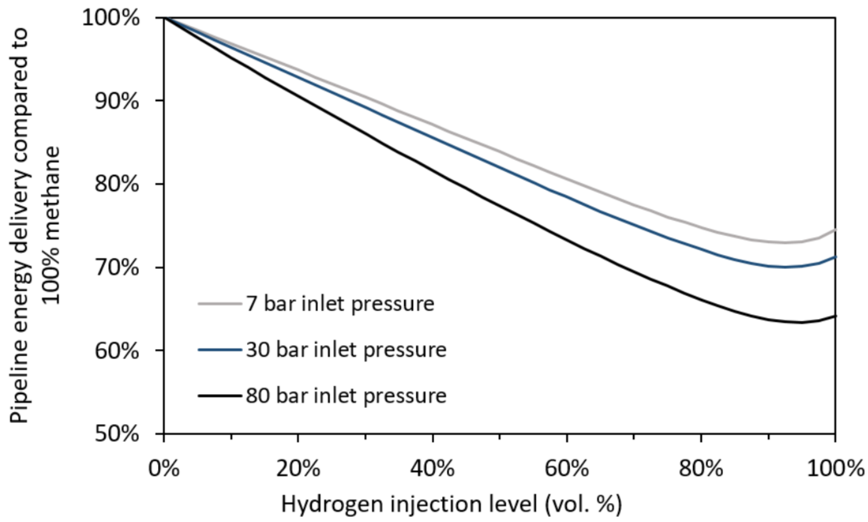


Figure 5-3: **Effect of hydrogen injection on natural gas pipeline energy delivery at three pressure levels.** Calculated by the authors using the general gas flow equation, assuming smooth pipe flow.

flow rates and linepack swing ranges for the pressure levels modelled. These results are shown in Figure 5-4, and further details can be found in the supplementary material. For a high pressure (80 bar) transmission pipeline, available linepack flexibility with 100% hydrogen is only around 17% of the equivalent value with natural gas. For a lower pressure (30 bar) pipeline, the available linepack flexibility is around 26%.

It may be possible to mitigate the poorer energy delivery and linepack performance of pipelines with hydrogen injection by adjusting the operating conditions (i.e. increasing pressure levels). However, this will depend on the practicality and safety of doing so.

5.2.2.2 Equipment operability

The differing properties of hydrogen also affect the usability of equipment on the gas grid and at end-use. Compressor stations, for example, are used on high pressure transmission networks to drive the flow of the gas. However, due to the considerably lower energy density of hydrogen, certain types of compressor are unlikely to be able to deliver a sufficiently high energy throughput using hydrogen and would need replacing [15].

At the distribution level, metering the quantity of energy supplied to consumers becomes challenging when hydrogen is injected partially and variably into gas supplies. Gas meters typically measure the volume of gas consumed, with no measure of the cal-

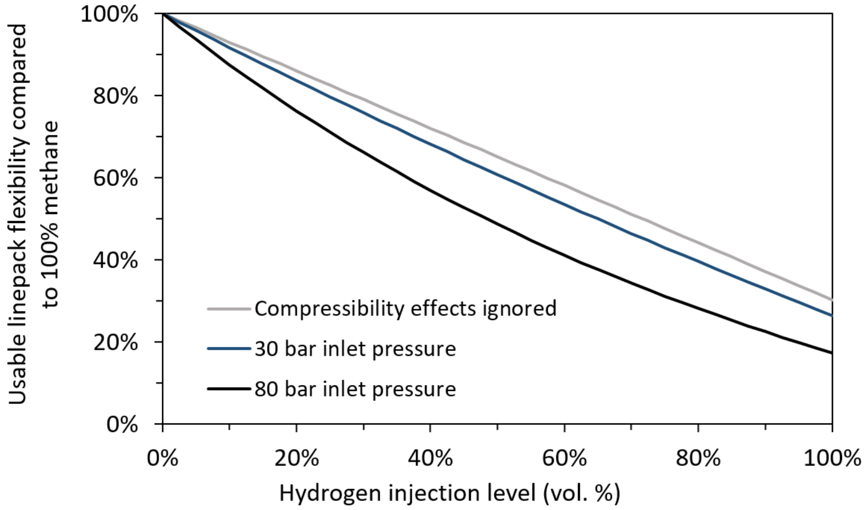


Figure 5-4: **Effect of hydrogen injection on usable pipeline linepack flexibility.** The energy content of a linepack swing between two fixed pressures was calculated for increasing levels of hydrogen injection. The linepack swing pressures were chosen to be representative of typical linepack swings for each pressure level.

orific value, but with hydrogen-natural gas blends the energy delivered per unit volume drops according to the amount of hydrogen present (cf. Figure 5-3). Thus, measuring volume consumed alone is not sufficient to determine energy consumption. These problems are already arising with increased levels of biomethane injection into gas grids, which also typically has a lower calorific value than natural gas. Methods are being investigated for tracking the energy delivered to consumers with gas of varying energy content, including through extensive measurement of gas calorific value throughout the gas grid, and modelling-based approaches [52].

End-use appliances would also be affected by hydrogen injection, primarily through reduced heat input, measured by the Wobbe index (equation 5.3), and flame speed. Various studies and testing programmes have been performed on domestic and industrial equipment for both partial hydrogen injection (e.g. [53, 54]) and complete conversion (e.g. [18]). It is likely that domestic equipment (e.g. natural gas boilers), could perform as normal under partial injection, up to a given limit (e.g. around 20 vol.%), but these appliances would need replacing for complete conversion to hydrogen [55].

Specialist industrial equipment such as gas turbines may be more sensitive to fuel composition, and therefore require more consideration. However, it is technically possible to operate gas turbines with any level of hydrogen-natural gas blend [56], and there are already many bespoke applications of turbines using hydrogen globally [57]. NOx emissions may be an issue for combustion of 100% hydrogen, but this can be mitigated, for example through water injection or lean pre-mixture combustion [58]. Beyond bespoke applications, turbine manufacturers have indicated that they will be able to supply hydrogen turbines at scale by 2030 [59]. Meanwhile, existing equipment can be retro-fitted for hydrogen or replaced, depending on costs.

5.2.2.3 Further safety and practical issues

Hydrogen embrittlement is a process where hydrogen diffuses into the existing flaws in steel and iron pipework, reducing the ductility of the material and increasing the likelihood of crack growth [29]. This is particularly a concern for the high-strength steels that are typically used in gas transmissions systems, and moreover higher pressures are thought to worsen the effects of embrittlement [29]. However, embrittlement is poorly understood, and various testing has found little or no reduction in performance of steel pipelines as a result of hydrogen embrittlement [49]. Furthermore, there are softer steels that are suitable for hydrogen at high pressures [49]. The literature is divided on the level of risk that embrittlement presents [60]; options may exist for mitigating these risks through further investment, such as rigorous pipeline inspection, or even retrofitting pipelines with hydrogen-resistant liners [5, 49]. The lower pressures on distribution systems mean that the risks of hydrogen embrittlement are lower. Furthermore, for lower pressures, more materials exist that are not susceptible to hydrogen embrittlement, such as polyethylene. In the UK, for example, much of the old hard steel and iron pipework on the distribution system is already being replaced as part of the Iron Mains Replacement Program [61].

Volumetric losses of hydrogen by leakage through pipe walls are larger than for natural gas, however energetic losses are lower, due to the lower energy density of hydrogen. Calculations have shown that volumetric losses through leakage for a hydrogen pipeline should be less than 0.001% of throughput [15]. Although not well understood, hydrogen is thought to behave as an indirect greenhouse gas, and it has been estimated that it has a 100-year global warming potential of around 4.3 [62]. However, for the very low levels of hydrogen leakage that would be expected, this would have a minimal overall global warming impact.

Certain properties of hydrogen raise concerns about the safety of using it as a replacement for natural gas. For example, hydrogen has a wider flammability range than natural gas, and lower limiting oxygen for combustion [49]. Partial mixing of hydrogen with natural gas would result in lower safety risks than use of pure hydrogen. Various testing and studies have been performed to assess the safety of using hydrogen in homes, including through the NaturalHy [17], GRHYD [63] and HyDeploy [54] projects. In the UK, a project is currently underway as part of the Hy4Heat programme to establish a full safety case for the use of 100% hydrogen in homes [18].

Some logistical issues arise when considering hydrogen injection, particularly for the case of partial injection. At the transmission level, transmission networks span different regions, and feed a variety of users including heavy industry, gas-fired power plants, and the local distribution networks. If hydrogen were to be injected into these systems, all users on the system would have to receive the hydrogen-natural gas blend, when in fact some facilities may require a "pure" natural gas feedstock. For example, in a high-hydrogen system, it is possible that some hydrogen will be produced from reforming natural gas; these reformers would benefit from the existing, unmodified natural gas transmission system.

In many countries, legislation would also have to be updated for hydrogen to be injected into gas grids. Much existing legislation is out-dated, with arbitrarily low specifications for the allowable level of hydrogen in the gas grid. In the UK, for example, the allowable limit is only 0.1 vol.%; in France the allowable limit is 6 vol.%; and in the Netherlands it is 12 vol.% [39].

5.2.2.4 Costs

Upgrade and conversion costs for injecting hydrogen into gas grids are uncertain, as there is limited practical experience of doing so. Nonetheless, some estimates have been made for the costs of injection equipment, gas grid upgrades, and preparation of homes for partial or complete conversion of gas grids to hydrogen.

A key argument for partial hydrogen injection is that limited upgrades would be required, meaning that costs would be low. Therefore the primary costs for partial injection would be safety checks on existing equipment, and installation of injection equipment. The HyDeploy project, demonstrating the feasibility of hydrogen injection at up to 20 vol.% into a private gas network with a peak gas demand of around 25 MW, estimate investment costs for site preparation of £655,000, giving an overall investment cost of around £26 per kW of gas grid capacity [54]. The injection equipment, including 500 kW electrolyser, is estimated at £1,900,000. However, the HyDeploy project is a demonstration project, and it is likely that costs would be lower at a larger scale. The HyNet project, which plans hydrogen production for a range of applications including injecting hydrogen into the gas grid at up to 20 vol.%, plans four injection sites, each supplying a peak gas demand of around 1400 MW [47]. Their estimated cost for each site is £5,000,000, meaning a cost of around £3.60 per kW of gas grid capacity.

For complete conversion of gas distribution grids to hydrogen, network upgrades are more extensive. The pipeline infrastructure would need to be surveyed and potentially upgraded to ensure that it is suitable for carrying 100% hydrogen. Furthermore, it is likely that pipelines may need to be reinforced in order to have sufficient peak energy delivery and linepack. However, arguably the injection and network monitoring requirements may be lower in a system that uses an unvarying gas supply (rather than partial, variable hydrogen injection). In the H21 project, in which the complete conversion of the gas distribution networks of the north of England was planned, the total capital costs for the conversion of the 42 GW peak capacity distribution system was estimated to be £143,000,000 [46]. This equals a conversion cost of £3.40 per kW of gas grid, divided equally between network reinforcement costs and the costs for the sectorisation of the network required to carry out the incremental switchover of the system. However, whilst this study includes thorough analysis of the capacity of the networks, it does not apportion costs for the surveying and safety checks of the pipelines, instead assuming that the ongoing Iron Mains Replacement Programme in the UK will ensure that all pipes on the networks will be converted to polyethylene already.

Meanwhile, consumer equipment that uses natural gas (for heating and cooking in domestic, commercial and industrial applications) would need at least upgrading and more likely replacing. Cost estimates for replacing natural gas heating systems with hydrogen in homes range between £1000 and £4000 per home [46, 55, 64, 65]. For non-domestic applications, costs vary significantly depending on the application, but are estimated to be in the region of £200 to £800 per kW capacity [46, 66].

5.2.3 Summary

In summary, hydrogen injection into existing gas grids offers an opportunity to create a reliable demand for hydrogen, which can help a larger hydrogen supply chain to develop whilst also reducing GHG emissions. Furthermore, the extent and flexibility of gas grids mean that hydrogen injection can provide benefits to the wider energy system, such as adding flexibility to the electricity system. However, the transport and flexibility capacities of natural gas infrastructures will be reduced when carrying hydrogen.

There are some practical and technical issues for hydrogen injection, but there is growing evidence that these can be overcome. Partial injection of hydrogen into gas distribution networks seems feasible and achievable. In the longer-term, conversion of distribution networks completely to hydrogen is also likely to be feasible, but this will be a much larger undertaking, due to the need to convert the majority of end-use equipment, including in homes. The feasibility of using existing high pressure transmission networks with hydrogen is less clear, as the same practical issues tend to be more severe when operating at higher pressures. There are also logistical reasons for keeping natural gas transmission networks in operation.

An alternative to using existing natural gas grids with hydrogen could be to build purpose-built hydrogen infrastructures. Purpose-built pipelines for hydrogen transmission could be advantageous, as they would be designed specifically for hydrogen, whilst existing natural gas pipelines would be kept intact. For distribution, brand new networks could be built in certain applications, such as at new-build residential or commercial sites, but it is unlikely to be realistic to build new distribution networks for existing buildings.

Importantly, building new hydrogen pipeline infrastructures will incur higher investment costs than converting existing infrastructures. This is a particular advantage of using existing infrastructures, as they can either be used partially (i.e. through partial injection) or converted gradually, meaning that infrastructure costs will not significantly outweigh hydrogen demand in the early stages of development.

The main alternative to pipeline transportation for hydrogen is transportation on road, typically with trucks carrying liquid or compressed gaseous hydrogen. This option is more straightforward at smaller scales, and is much more logistically flexible, but it becomes more costly for larger hydrogen volumes and transportation distances [67]. Furthermore, this option does not include the benefits of a steady hydrogen supply or gas grid linepack.

A further advantage of purpose-built infrastructures (pipeline or road transport) is that it would be easier to control hydrogen purity. Whilst hydrogen purity is less important for combustion, in fuel cell applications (either stationary or in vehicles) high hydrogen purity is required, and re-purposed natural gas pipelines may be unable to supply this [57].

5.3 Method

In order to explore the role of gas grids and hydrogen in helping to deliver low carbon energy systems, a value chain optimisation model was developed of a national energy system. The Great Britain (GB) energy system was chosen, as it represents a large sized energy system with heavy reliance on natural gas grids.

5.3.1 Model

The value chain optimisation was carried out using the Value Web Model (VWM), developed by Samsatli and Samsatli [68]. In this study, the representation of resource transmission and distribution networks in the VWM was extended. This included modelling of linepack storage on both the gas transmission and distribution networks, and the ability to inject hydrogen into existing gas distribution grids. An overview of the VWM is provided in section 5.3.1.1, and sections 5.3.1.2 to 5.3.1.4 describe the additions that were made to the model in this work, including the new mathematical constraints. A reduced nomenclature, covering the equations presented in this work, is provided in appendix B[†]. The full model mathematical formulation and nomenclature can be found in previous studies by Samsatli and co-workers (e.g. [68, 69, 70]).

5.3.1.1 Overview of the Value Web Model

The VWM is a mixed integer linear programming (MILP) optimisation model that can be used to optimise the value chains in an energy system. The model includes a variety of energy technologies and resources, and has a spatio-temporal representation. Spatially, the model includes discrete zones (16 different zones in the case of GB), each of which has its own resource availabilities and demands. Temporally, the model represents time intervals at four different scales: sub-day intervals can represent the hourly variability in demands and availabilities of resources; day-type intervals can be used, e.g. for different demand profiles on weekdays and weekends; seasonal intervals are used to represent difference in resource demand and availability throughout the year; and finally long-term planning intervals are included for long-term changes in demands as well as long-term technology investment decisions.

An illustration of the structure of the VWM is provided in Figure 5-5. The model includes availability of primary resources (e.g. natural gas, solar and wind, shown in circles in Figure 5-5). These resources can be converted to other resources within the energy system via conversion technologies (shown as rectangles). Different types of conversion technologies exist, including those that directly utilise primary resources (e.g. wind turbines and solar PV), general "industrial" conversion technologies (e.g. electrolysers and gas turbines), distribution technologies (e.g. gas and electricity distribution

[†]This original article appendix is not included in this thesis, but a full nomenclature for the model is provided in Appendix A of the thesis.

networks), and domestic and commercial technologies that utilise these distributed resources. All of the resources included in the VWM are shown in Figure 5-5 (as circles); all of the resource conversions are represented with arrows connecting resources to technologies. Each technology may consume or produce more than one resource; key parameters for each technology are defined, including costs, rates of resource conversion (i.e. efficiency), and maximum operating rates. In addition to the description provided here, more information about the technologies and resources included in the VWM can be found in the associated Data in Brief article [71], which provides an overview of all of the model input data used in this study.

Many resources are included in different forms within the VWM, so that the associated processes can be modelled. For example, CO_2 is represented as "emitted", "captured" and "stored", with conversion technologies to convert between each of these states. Similarly, natural gas and hydrogen are both represented at "low pressure" (i.e. transmission-level pressure), "high pressure" (for storage at around 200 bar), and as a "distributed" gas. Distribution technologies are included in the VWM for the first time in this work. Distribution technologies are a subset of conversion technologies, that convert "centralised" resources such as electricity or gas from the transmission system to "distributed" resources to be used in homes and businesses. These technologies have a fixed size, representative of a portion of the distribution network, but multiple instances of the technology can be installed within one zone. In this way, the costs and constraints of distribution infrastructures are included. Representation of gas distribution networks includes the linepack storage capacity of these networks and the ability to inject hydrogen (either partially or as a complete conversion). More details of this modelling are provided in section 5.3.1.3.

Some resources may have demands associated with them that must be satisfied; in this study, demands for electricity and heat are included. Heat demands are separated into three groups: domestic heat, commercial heat (including low-temperature industrial heat), and high temperature industrial heat. This allows representation of the different types of heating technologies that exist, such as domestic boilers in homes, commercial heating for larger buildings, and specialised equipment for industry (e.g. furnaces). Heat from commercial heating can also be delivered to homes (i.e. converted to domestic heat) via a heat network (a distribution technology).

Two separate spatial zones are depicted in Figure 5-5. Conversion and storage technologies can be built in each zone, and transportation technologies exist that can move resources between zones (e.g. electricity transmission and gas pipelines, shown with hexagons in Figure 5-5). Some transportation technologies include storage capacity, to represent linepack; more details of this are provided in section 5.3.1.2. Specific storage technologies are also modelled (e.g. pressure vessels and underground storage, shown with pentagons in Figure 5-5), and resources can be loaded into storage, to be extracted during a later time interval.

All technologies have impacts associated with their installation and operation, such as costs and environmental impacts. The model is able to determine the optimal configuration of technologies (e.g. when and where they should be built), and how these technologies should be operated, in order to satisfy the final energy demands. The objective function to optimise can be cost-based (e.g. minimise overall system cost), or can take into account other objectives. In addition to the numerous constraints in the VWM that ensure that resource flows are in balance and that technologies operate within their feasible limits, further constraints can be included such as limits on GHG emissions.

5.3.1.2 Gas transmission

"Transmission" is used to refer to the high pressure pipelines that transport gas around the country; in the VWM, this equates to transportation of gas between the discrete spatial zones of the model. To represent the storage and transportation capability of gas transmission systems, a single technology type ("national infrastructure") is defined for all spatial zones in the model. This is modelled as a single storage technology for the whole of GB (or whichever country or region is being modelled) that allows any zone connected to it (via pipelines) to inject or withdraw resource, as shown in Figure 5-6. Thus transmission occurs by injecting resource from one zone and withdrawing from another; linepack is increased if the total (over all zones) rate of injection of resource is greater than the total rate of withdrawal. Therefore the constraints required to model gas transmission with linepack storage are the same as those for regular storage technologies, as presented by Samsatli and Samsatli [68, 72, 73], with the following differences: there is a single inventory of stored resource (independent of zone) and a single associated "hold" task; and there is a "put" and "get" task for each zone connected to the transmission network, allowing each zone to inject and withdraw resource from the network. The constraints for the transmission network with linepack storage are described below.

The net flow of resource (i.e. gas) out of the transmission infrastructure, into each

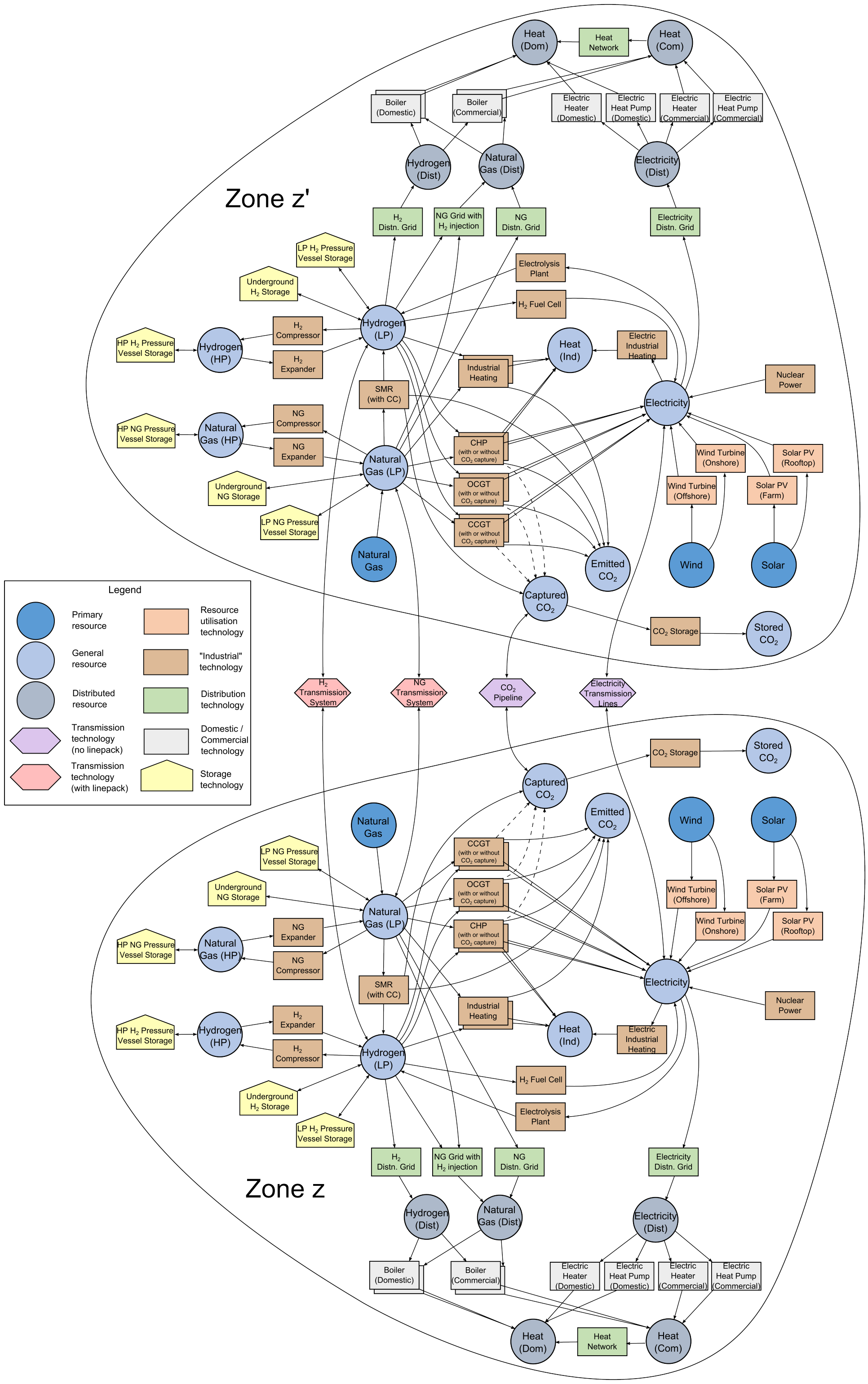


Figure 5-5: **Representation of resources and technologies in the Value Web Model.** Different resource types include primary, general energy system, and distributed. Various technology types exist that can convert between these resources. Also represented in the model are transportation and storage technologies.

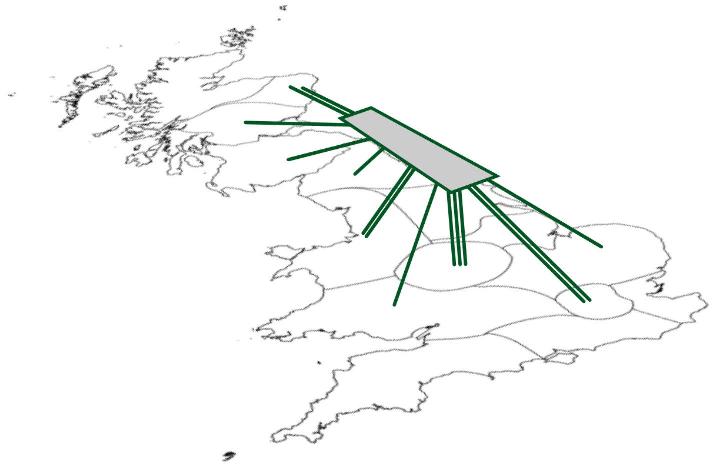


Figure 5-6: **Representation of gas transmission systems in the Value Web Model.** Pipelines (green lines) can be built in any zone, connecting the zone to the national transmission system. Any zone with a connecting pipeline can inject or withdraw gas from the system. Multiple pipelines can be built for increased injection and withdrawal rates. The overall storage capacity of the system (linepack) is determined by the total number of pipelines built.

spatial zone is tracked using "put", "hold" and "get" tasks:

$$L_{zrhdty} = \sum_{l} \left(\mathscr{L}^{\text{put}}_{lzhdty} \lambda^{\text{put}}_{lr,\text{src},y} + \mathscr{L}^{\text{get}}_{lzhdty} \lambda^{\text{get}}_{lr,\text{dst},y} \right) \tag{5.4}$$

$$\forall r \in \mathbb{R},\ z \in \mathbb{Z},\ h \in \mathbb{H},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y}$$

L_{zrhdty} is the net flow of resource from the transmission infrastructure l into a zone z. The net flow is negative if resource is being added to the transmission system (linepack increased), or it is positive if the linepack is being depleted. Different zones may be adding or removing resource from the transmission infrastructure at one time, allowing for transportation of resource between zones. The "put" and "get" tasks are used to model costs and energy requirements associated with adding resource to the infrastructure and taking from it, respectively. Each of these tasks has a conversion factor, $\lambda^{\star}_{lrfy}$ ($\star \in$\{put, hold, get\}), which is multiplied by the operation rate of the respective task ($\mathscr{L}^{\text{put}}_{lzhdty}$, $\mathscr{L}^{\text{hold}}_{lhdty}$ and $\mathscr{L}^{\text{get}}_{lzhdty}$) to give the flow rate of the resource into and out of the transmission infrastructure. The "hold" task represents the maintenance of resource in storage (i.e. the linepack in the whole network), as described later and seen in equations 5.7 to 5.9. The set of linepack transmission infrastructures in the model ($l \in \mathbb{L}$) includes natural gas transmission infrastructures and hydrogen transmission infrastructures (other transmission systems, without linepack, are modelled separately).

The other sets shown in equation 5.4 represent the set of resources ($r \in \mathbb{R}$, including all of the resources shown in Figure 5-5), set of spatial zones ($z \in \mathbb{Z}$), and various time intervals. Definitions of each of these sets are provided in the nomenclature in appendix B‡.

The operation rates of the "put" and "get" tasks can vary in time (indicated by the h, d, t and y indices representing hourly, day-type, seasonal and annual time intervals, respectively), and are also dependent on the spatial zone, z. Pipelines must be built in a zone for it to be connected to the national infrastructure. Each pipeline has a fixed maximum transportation rate, which determines the rate at which the resource can be injected into or withdrawn from the transmission system (denoted by $l_l^{\text{put,max}}$ and $l_l^{\text{get,max}}$ respectively). Multiple pipelines can be built in a given zone in order to increase the withdrawal/injection rate. Thus, the maximum rate at which resource can be transferred between the transmission infrastructure and a spatial zone is given as follows:

$$\mathscr{L}_{lzhdty}^{\text{put}} \leq N_{lzy}^{\text{L}} l_l^{\text{put,max}} a_{lz} \qquad \forall l \in \mathbb{L},\ z \in \mathbb{Z},\ h \in \mathbb{H},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y} \quad (5.5)$$

$$\mathscr{L}_{lzhdty}^{\text{get}} \leq N_{lzy}^{\text{L}} l_l^{\text{get,max}} a_{lz} \qquad \forall l \in \mathbb{L},\ z \in \mathbb{Z},\ h \in \mathbb{H},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y} \quad (5.6)$$

Where N_{lzy}^{L} is the number of pipelines built connecting zone z to the transmission system l and a_{lz} is a parameter that can be set to 0 or 1 to specify whether a zone may connect to the transmission system. The number of pipelines built in all zones also determines the overall storage capacity of the transmission infrastructure (this will be defined and explained later, in equation 5.18).

In reality, gas transmission systems are complex, spanning a varied landscape with a range of different pipeline lengths, diameters and operating regimes. The approach used here, in which each pipeline has the same diameter, length, maximum flow rate and linepack flexibility, is a simplification. For example, this representation assumes that all zones can connect to the same transmission system for the same cost, regardless of distance from the remainder of the transmission system. However, this approach enables modelling of both the storage and transportation capabilities of a gas transmission system with minimal complexity. Furthermore, with appropriate data assumptions, the overall operating regime of the system (e.g. maximum transportation rates and

‡This original article appendix is not included in this thesis, but a full model nomenclature is provided in Appendix A of the thesis.

linepack swing) can be modelled accurately.

A series of equations are used in the VWM to manage the overall linepack inventory of the transmission system. The overall linepack inventory, J_{lhdty}, is based on the flows of resource into and out of the system, as follows:

$$J_{lhdty} = n_h^{\text{hd}} \sum_r \left(\sum_z \mathscr{L}_{lzhdty}^{\text{put}} \lambda_{lr,\text{dst},y}^{\text{put}} + \mathscr{L}_{lhdty}^{\text{hold}} \lambda_{lr,\text{src},y}^{\text{hold}} + \sum_z \mathscr{L}_{lzhdty}^{\text{get}} \lambda_{lr,\text{src},y}^{\text{get}} \right) \tag{5.7}$$
$$\forall l \in \mathbb{L},\ h \in \mathbb{H},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y}$$

The rate of operation of the "hold" task is defined as the current linepack level divided by the length of the time interval:

$$\mathscr{L}_{l,1,dty}^{\text{hold}} = J_{ldty}^{0,\text{sim}} / n_1^{\text{hd}} \qquad \forall l \in \mathbb{L},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y} \tag{5.8}$$

$$\mathscr{L}_{lhdty}^{\text{hold}} = J_{l,h-1,dty} / n_h^{\text{hd}} \qquad \forall l \in \mathbb{L},\ h > 1 \in \mathbb{H},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y} \tag{5.9}$$

The daily linepack "surplus" is the change in linepack inventory between the first and last hourly intervals of the day type d:

$$\Delta_{ldty}^{\text{d}} = J_{l,|\mathbb{H}|,dty} - J_{ldty}^{0,\text{sim}} \qquad \forall l \in \mathbb{L},\ d \in \mathbb{D},\ t \in \mathbb{T},\ y \in \mathbb{Y} \tag{5.10}$$

The surplus for a week in season t is then calculated from the sum of the daily surpluses of each day type d in the given week, accounting for the number of repetitions of each day type n_d^{dw}:

$$\Delta_{lty}^{\text{t}} = \sum_d \Delta_{ldty}^{\text{d}} n_d^{\text{dw}} \qquad \forall l \in \mathbb{L},\ t \in \mathbb{T},\ y \in \mathbb{Y} \tag{5.11}$$

Finally, the surplus over year y is the sum of all seasonal surpluses:

$$\Delta_{ly}^{\text{y}} = \sum_t \Delta_{lty}^{\text{t}} n_t^{\text{wt}} \qquad \forall l \in \mathbb{L},\ y \in \mathbb{Y} \tag{5.12}$$

A constraint is also included to keep the linepack over one year stationary (i.e. no yearly linepack surplus or deficit; this could also be applied on a shorter timescale if required):

$$\Delta^{\mathrm{y}}_{ly} = 0 \qquad \forall l \in \mathbb{L},\, y \in \mathbb{Y} \tag{5.13}$$

The linepack inventory must be tracked to ensure that it does not exceed or fall below its allowable operational levels, and so that the impacts (e.g. costs) and resource requirements of holding linepack inventory are correctly accounted for. However, rather than explicitly calculating the inventory based on resource flows for each hourly interval of the entire time horizon, the total impacts and resource requirements can be calculated from the "average" inventory profile for each day type, season and yearly period. The "average" inventory profile that will give the same overall impacts and resource requirements as the full inventory profile is calculated from the initial linepack inventory at the beginning of each new time interval type, $J^{0,\mathrm{act}}_{ldty}$, and the time interval surpluses defined in equations 5.10 to 5.12:

$$J^{0,\mathrm{sim}}_{ldty} = J^{0,\mathrm{act}}_{ldty} + \left[\left(n^{\mathrm{dw}}_{d} - 1\right)\Delta^{\mathrm{d}}_{ldty} + \left(n^{\mathrm{wt}}_{t} - 1\right)\Delta^{\mathrm{t}}_{lty} + \left(n^{\mathrm{yy}}_{y} - 1\right)\Delta^{\mathrm{y}}_{ly}\right]/2 \qquad \forall l \in \mathbb{L},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{5.14}$$

The initial linepack inventory for each new time interval type is calculated from the linepack at the beginning of the previous time interval type, plus the linepack surplus accumulated over the course of the previous time interval type. This approach is used for each new day type, season, and planning period:

$$J^{0,\mathrm{act}}_{ldty} = J^{0,\mathrm{act}}_{l,d-1,ty} + n^{\mathrm{dw}}_{d-1}\Delta^{\mathrm{d}}_{l,d-1,ty} \qquad \forall l \in \mathbb{L},\, d > 1 \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{5.15}$$

$$J^{0,\mathrm{act}}_{l,1,ty} = J^{0,\mathrm{act}}_{l,1,t-1,y} + n^{\mathrm{wt}}_{t-1}\Delta^{\mathrm{t}}_{l,t-1,y} \qquad \forall l \in \mathbb{L},\, t > 1 \in \mathbb{T},\, y \in \mathbb{Y} \tag{5.16}$$

$$J^{0,\mathrm{act}}_{l,1,1,y} = J^{0,\mathrm{act}}_{l,1,1,y-1} + n^{\mathrm{yy}}_{y-1}\Delta^{\mathrm{y}}_{l,y-1} \qquad \forall l \in \mathbb{L},\, y > 1 \in \mathbb{Y} \tag{5.17}$$

Finally, constraints are included to ensure that the linepack inventory always remains within its operational limits. The maximum and minimum allowable linepack inventories for the entire transmission system are the upper and lower bounds of the following equation, and are calculated from the maximum and minimum allowable inventories for a single pipeline, and the total number of pipelines installed in all zones. Due to the repeated time intervals within each time interval type (e.g. repeated days within a week), the maximum and minimum linepack inventories will always occur in the first or last interval of an interval type. Therefore only these intervals need to be constrained. The first and last intervals of each day, season and planning period each must be constrained, resulting in 8 different constraints, which is then doubled to 16 to account for both the lower and upper bounds on the linepack inventory. These 16 constraints are shown in shorthand below, where all 8 combinations of plus and minus should be considered:

$$l_l^{\text{hold,min}} \sum_z N_{lzy}^{\text{L}} a_{lz} \leq J_{lhdty} \pm G_{ldty} \leq l_l^{\text{hold,max}} \sum_z N_{lzy}^{\text{L}} a_{lz} \tag{5.18}$$
$$\textit{where} \qquad G_{ldty} = \frac{\left(n_d^{\text{dw}} - 1\right) \Delta_{ldty}^{\text{d}} \pm \left(n_t^{\text{wt}} - 1\right) \Delta_{lty}^{\text{t}} \pm \left(n_y^{\text{yy}} - 1\right) \Delta_{ly}^{\text{y}}}{2}$$
$$\forall l \in \mathbb{L},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y}$$

As with all technologies installed in the model, the total number of pipelines installed in a given zone z in a given planning period y is tracked based on the number of pre-existing pipelines, N_{lz}^{EL}; number of pipelines installed, NI_{lzy}^{L}; and number of pipelines and pre-existing pipelines retired (NR_{lzy}^{L} and NR_{lzy}^{EL}):

$$N_{lzy}^{\text{L}} = \begin{cases} N_{lz}^{\text{EL}} + NI_{lzy}^{\text{L}} - NR_{lzy}^{\text{L}} & \forall l \in \mathbb{L},\, z \in \mathbb{Z},\, y = 1 \\ N_{lz,y-1}^{\text{EL}} + NI_{lzy}^{\text{L}} - NR_{lzy}^{\text{L}} - NR_{lzy}^{\text{EL}} & \forall l \in \mathbb{L},\, z \in \mathbb{Z},\, y > 1 \end{cases} \tag{5.19}$$

The number of pipelines retired is calculated from the technical lifetime of the pipeline.

For the practical reasons described in section 5.2.2, injection of hydrogen (either partial or complete conversion) into existing natural gas transmission pipelines was not modelled as an option. Instead, separate hydrogen transmission pipelines must be built. These have the same linepack capabilities as the equivalent natural gas system (although with lower energy throughput and storage).

5.3.1.3 Gas distribution

"Distribution" is used to refer to the delivery of gas from centralised locations such as storage facilities or the transmission system to the homes and businesses that use it for heating. Hydrogen distribution networks have previously been modelled in the VWM (e.g. [69, 74]) but this work is the first time that electricity and natural gas distribution networks have also been modelled. More importantly, the linepack capability of the natural gas and hydrogen distribution networks has now been modelled, as well as hydrogen injection into the natural gas distribution network and the option to convert to pure hydrogen networks. In order to represent both the delivery of gas to consumers and the storage capability (linepack) of distribution systems, they are represented in the model by a conversion technology coupled to a storage technology. An illustration of how these networks are represented is shown in Figure 5-7. Figure 5-7(a) shows the modelling of a conventional gas distribution grid (with linepack), whilst Figures 5-7(b) and 5-7(c) show operation with partial hydrogen injection and complete conversion to hydrogen, respectively.

All conversion technologies in the model, including for distribution technologies and other conversion technologies such as gas turbines or electrolysers are governed by the following constraint, defining the net rate of production (or consumption) of resource r:

$$P_{rzhdty} = \sum_{p \in \mathbb{P}} \mathscr{P}_{pzhdty} \alpha_{rpy} \qquad \forall r \in \mathbb{R},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \tag{5.20}$$

where P_{rzhdty} is the net resource production rate, $\mathscr{P}_{pzhdty}$ is the operating rate of the technology and α_{rpy} is a conversion factor that defines the rate of conversion between resources. For gas distribution networks this represents a conversion of 1 MWh of "centralised" gas to 1 MWh of "distributed" gas and can also include other resource requirements, such as electricity requirements for the process.

All conversion technologies, including distribution networks, come in pre-defined sizes in the model, but several of these technologies can be installed in one zone in order to increase the maximum overall operating rate. Hence, the overall operating rate of a technology type p in a zone z is constrained by upper and lower bounds based on the allowable operating rates of a single technology ($p_p^{\max}$ and $p_p^{\min}$) and the number of

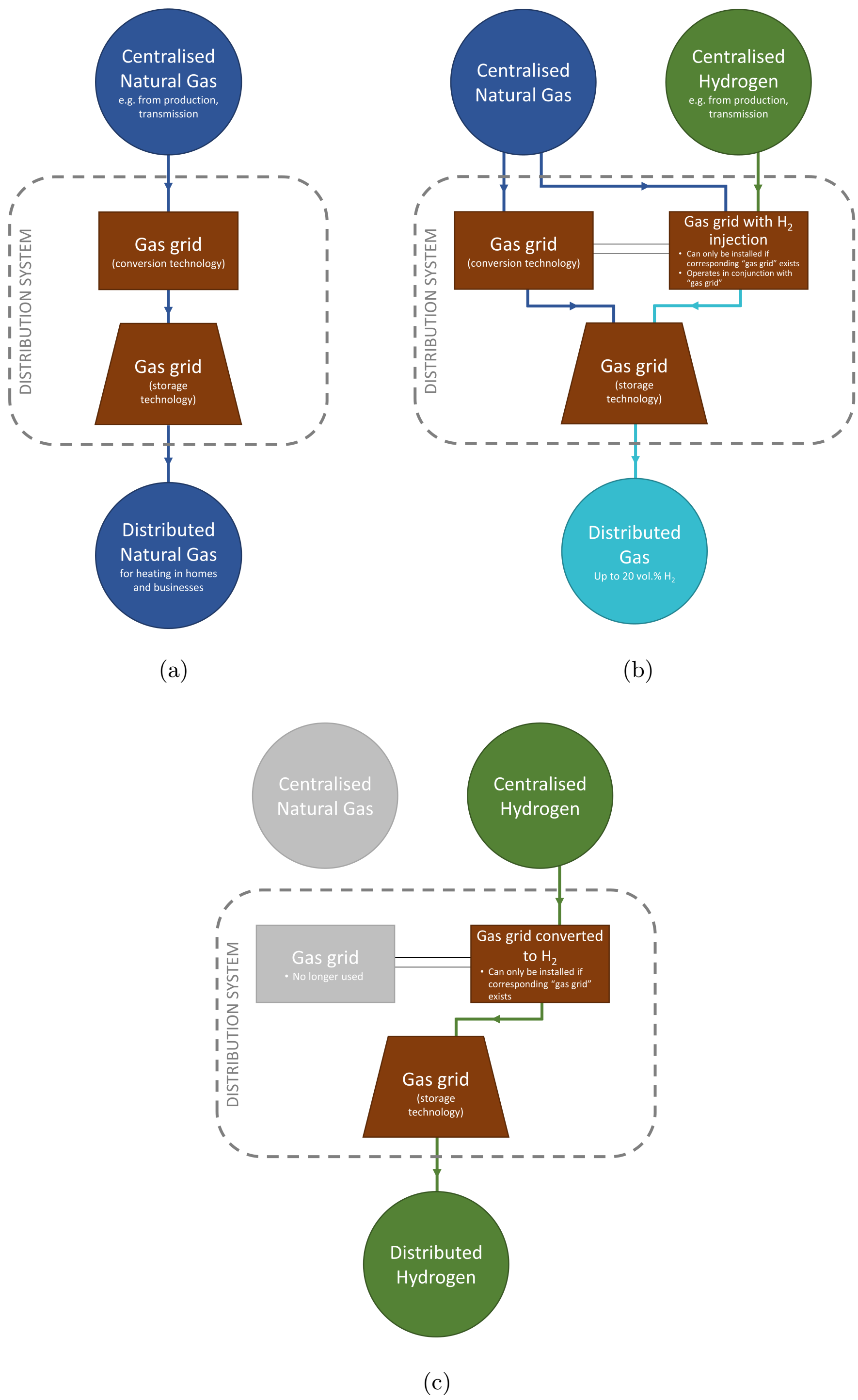


Figure 5-7: **Representation of gas distribution networks in the model.** (a) Standard natural gas distribution grid, including conversion of "centralised" gas to "distributed" gas, and storage (linepack) capacity of the grid; (b) Partial hydrogen injection into an existing natural gas grid; (c) Complete conversion of an existing natural gas grid to hydrogen.

technologies installed (N^{PC}_{pzy}):

$$N^{\mathrm{PC}}_{pzy} p^{\min}_{p} \leq \mathscr{P}_{pzhdty} \leq N^{\mathrm{PC}}_{pzy} p^{\max}_{p} \qquad \forall p \in \mathbb{P},\, z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y} \quad (5.21)$$

The total number of conversion technologies installed in a zone is tracked in the same manner as for the linepack technologies, as shown in equation 5.19. With this representation, all of the costs, efficiencies and operating rates of the gas distribution grid are represented in the model. As shown in Figure 5-7(a), in order to represent the gas distribution grid linepack, a storage technology is coupled to the conversion technology. In general, storage technologies are modelled in a similar manner to the linepack technology constraints shown in equations 5.4 to 5.19, except that separate storage technologies can be built in each zone, rather than only one national infrastructure, and the zones can only have access to their own storage technologies (rather than any zone that is connected to the national infrastructure). For the full mathematical formulation for storage technologies, refer to [68, 69].

The storage technology representing distribution grid linepack has zero cost (this is included in the conversion technology), but represents the storage capacity of the distribution grid. The storage capacity of each portion of distribution grid was determined based on UK data for the overall linepack capacity of the gas distribution system [43], and estimates of the peak delivery rate of the distribution system from National Grid data [6]. Distribution grid conversion and storage technologies must always be installed together, therefore a constraint is included that the number of each is equal:

$$N^{\mathrm{S}}_{szy} = N^{\mathrm{PC}}_{pzy} \qquad \forall s \in \mathbb{S}^{\mathrm{Dist}},\, z \in \mathbb{Z},\, y \in \mathbb{Y},\, p \in \mathbb{P}^{\mathrm{Dist}},\, SP_{sp} = 1 \qquad (5.22)$$

where SP_{sp} is an association parameter that is equal to 1 where a storage technology is associated with a conversion technology (i.e. the corresponding storage and conversion technologies for the distribution network in question), and equal to 0 otherwise.

This representation is available for both natural gas distribution networks and for hydrogen distribution networks (if the model chooses to build these). Additionally, hydrogen injection into existing natural gas networks is modelled. Two options for injection of hydrogen into gas grids are modelled: partial, variable injection up to a level of 20 vol.%, or complete conversion of networks to hydrogen.

Figure 5-7(b) illustrates how partial hydrogen injection is represented in the VWM, using a conversion technology that converts natural gas and hydrogen in a fixed ratio (80:20 by volume / 93:7 by energy) into the same "distributed" gas that a typical natural gas distribution grid converts natural gas into. This technology can operate at a variable rate, alongside existing gas distribution grid technologies, so that the average hydrogen injection rate in the zone is determined by the relative operating rates of the technologies.

Figure 5-7(c) illustrates how complete conversion of a portion of gas distribution grid to hydrogen is represented in the VWM, using a new conversion technology that, similar to a new hydrogen distribution grid, converts "centralised" hydrogen to "distributed" hydrogen. However in this case, a "complete conversion" technology replaces an existing conventional gas distribution technology, (i.e. the section of gas distribution grid has been switched from natural gas to hydrogen and cannot be switched back). A constraint is included to ensure that the number of "complete conversion" technologies installed cannot exceed the number of conventional gas grid technologies already installed:

$$N^{PC}_{HIGG-ComCon,zy} \leq N^{PC}_{NG\,DistGrid,zy} \qquad \forall z \in \mathbb{Z}\, y \in \mathbb{Y} \tag{5.23}$$

Finally, a constraint is required to ensure that the overall peak capacity of the gas distribution grid in a given zone is modified based on the number of partial hydrogen injection and complete conversions carried out. Converting a portion of the distribution grid to hydrogen reduces the total capacity for delivering natural gas. Meanwhile installation of a "partial injection" technology does not increase the peak capacity of gas delivery. Therefore, a constraint specifies that the overall operating rate of all conventional gas distribution and partial hydrogen injection technologies in a zone does not exceed the maximum allowable operating rate of the remaining gas grid (that has not undergone complete conversion to hydrogen).

$$\sum_{p \in \mathbb{P}^{\mathrm{HIGG}}} \mathscr{P}^{\mathrm{h}}_{pzhdty} \leq (N^{PC}_{NG\,DistGrid,zy} - N^{PC}_{HIGG-ComCon,zy}) p^{\max}_{NG\,DistGrid} \tag{5.24}$$

$$\forall z \in \mathbb{Z},\, h \in \mathbb{H},\, d \in \mathbb{D},\, t \in \mathbb{T},\, y \in \mathbb{Y}$$

Representing partial injection into the distribution grid and conversion of the distribution grid to 100% hydrogen as "partial injection" and "complete conversion" conversion technologies enables the optimisation to choose where and when these decisions may take place, taking into account the costs and other impacts of doing so.

Table 5.1: Details of the scenarios modelled.

Time horizon	Issues explored	Number of scenarios modelled
2020	Partial hydrogen injection	33
2050	Effect of CO_2 emissions targets	6
2050	Conversion of gas grids to hydrogen	14

5.3.1.4 Further additions

Electricity distribution networks were also included in the VWM. They are modelled by only a conversion technology as the electricity network has no linepack storage equivalent. Solar power was also included in the VWM for the first time in this work. Solar irradiance is included as a time-varying natural resource and solar PV technologies can be built to utilise this resource. Both rooftop and solar farm PV units can be installed, and have costs, efficiencies, and land footprint constraints associated with them.

5.3.2 Scenarios

In this study the VWM was applied to the GB energy system, as this represents a medium-sized energy system with an extensive gas grid, multiple energy resources (including wind, solar, nuclear, and natural gas), and stringent decarbonisation targets. The resources and technologies included in the optimisation are shown in Figure 5-5. The complete set of model input data used in this study, including resource availabilities and demands, and technology costs and operating data, can be found in the associated data article [71]. The optimisation objective was to satisfy overall demands for heat and electricity, including domestic, commercial and industrial demands, to maximise overall system net present value (NPV).

Table 5.1 provides a summary of the scenarios that were studied. Scenarios in both 2020 and 2050 were considered. In the 2020 scenarios, the present-day potential for partial hydrogen injection into the gas grid was investigated, including the effect of FITs incentivising the injection of hydrogen into the gas grid. For the 2050 scenarios, first the effects of different decarbonisation targets on the optimal energy system were assessed. Following this, the role of hydrogen in the optimal 2050 energy system was considered, focussing on the conversion of gas grids to hydrogen. The results and further details of these scenarios are provided in sections 5.4.1, 5.4.2.1 and 5.4.2.2.

Each of the 53 scenarios in Table 5.1 includes around 133,000 constraints and 77,000 variables, of which over 900 are integer variables. The optimisation was performed on a workstation with 10 cores and 128 GB RAM. Each scenario took up to three hours to solve with an optimality tolerance of 2%. Choices in scenario design will always be subject to some trade-offs with computational capability. For example, the size of the problem, hence the computational effort required, quickly scales up with the number of spatial zones or time intervals. The spatio-temporal resolutions used in the scenarios in this paper represent a good balance between achieving sufficient detail to answer the research questions posed without becoming computationally intractable.

5.4 Results: the role of hydrogen and gas grids in Great Britain

5.4.1 Opportunities for partial hydrogen injection today

A number of scenarios were modelled, exploring the role that hydrogen injection could have in the present day energy system, based on a hydrogen FIT incentivising injection into the gas grid. This tariff acts as a financial reward for every MWh of hydrogen that is injected partially into the natural gas distribution grid. Scenarios with FITs in the range of £0/MWh to £100/MWh were modelled. In order to carry out hydrogen injection, the injection equipment must be installed and relevant safety checks carried out; the costs of carrying out these upgrades were included in the capital cost of the "partial injection" technology. In the central case, these costs were assumed to be £3.60 per kW of gas distribution grid capacity, based on estimates from the HyNet project [47]. Sensitivity scenarios for these costs were also modelled, with upper and lower cost estimates of £7.20 and £1.80 per kW of grid capacity, respectively.

5.4.1.1 Effect of feed-in tariff on hydrogen uptake

Figure 5-8 shows the average level of partial hydrogen injection across the whole gas grid distribution network in each of the optimisation scenarios described above. As expected, higher FITs incentivise increased hydrogen injection. The upper limit for injection in these scenarios is 20 vol.%, which is a technical constraint based on the issues discussed in section 5.2. For higher levels of injection, the grid must be converted to 100% hydrogen, which would incur further costs and is not supported by a FIT in these scenarios.

In scenarios with FITs of up to £20/MWh, very low levels of hydrogen are injected

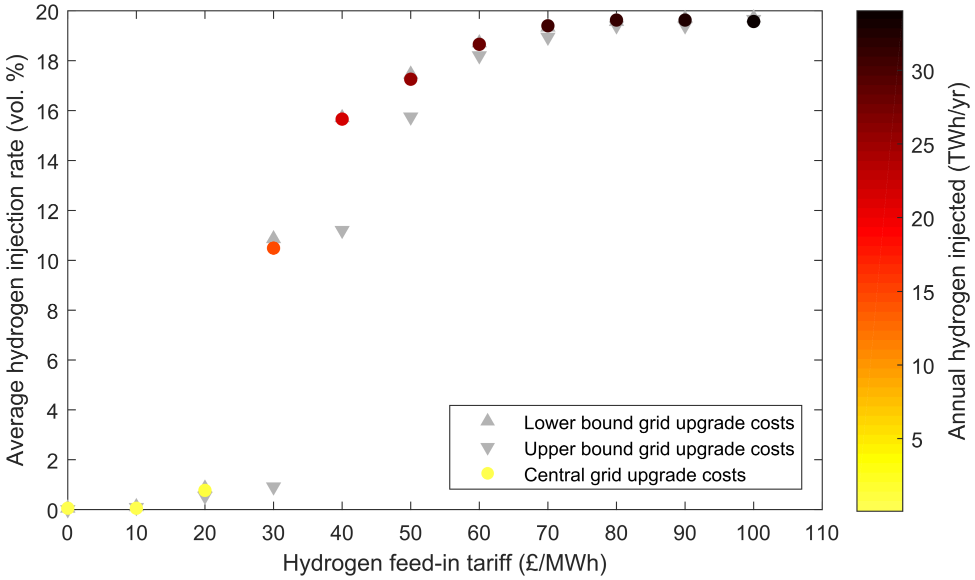


Figure 5-8: **Rate of partial hydrogen injection into the gas distribution grid in scenarios with a range of hydrogen feed-in tariffs and upgrade cost assumptions.** The average level of injection is the average across the entire gas distribution system. 20% injection in volume terms is equal to 7% in energy terms.

(less than 1 vol.% on average across the whole system). With no FIT in place, annual injection is 0.1 TWh/yr, rising to 1.0 TWh/yr in the case with a FIT of £20/MWh. In these scenarios, hydrogen is only a small part of the wider energy system, and all hydrogen is produced from power-to-gas.

Figure 5-9 (left) shows a map of the hydrogen-related technologies installed in the scenario with a FIT of £20/MWh. Electrolysers are installed in only four zones and are accompanied by some pressure vessel hydrogen storage. Hydrogen is mostly produced overnight, when excess electricity is available. Although the gas grid linepack allows for some flexibility, the storage vessels are installed so that hydrogen injection can be maximised throughout the day. Almost all hydrogen (96%) is injected into the gas distribution grid and the remainder is used directly for heating, for example in industrial plants that are connected directly to the hydrogen production or storage facilities.

With FITs of £30/MWh and above, there is sufficient incentive to build SMR plants, leading to a much larger scale of hydrogen production and higher levels of injection into the gas grid. However, the cost of injection also depends on the variability of gas demand and the flexibility of hydrogen supply. In the case with a FIT of £30/MWh, SMR plants are operated consistently throughout the year, producing a steady supply

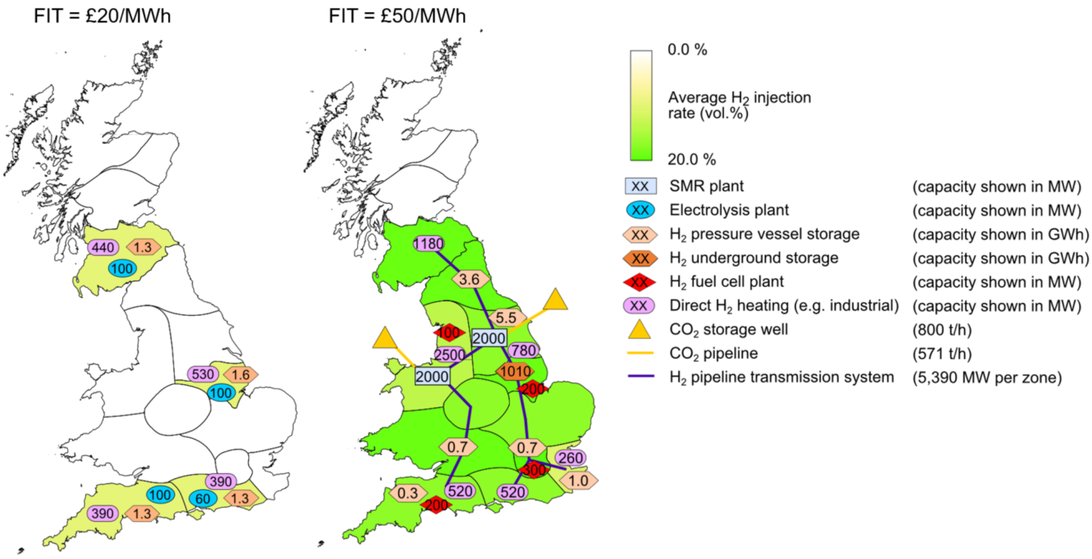


Figure 5-9: **Maps of the hydrogen-related technologies installed in two present-day scenarios with partial hydrogen injection.** The map on the left shows details of the power-to-gas based system arising in the case with a feed-in tariff of £20/MWh; the map on the right shows details of the SMR based system arising in the case with a feed-in tariff of £50/MWh. Only hydrogen-related technologies are shown: further technologies that are not shown in the figure include the existing natural gas transmission system and electricity generation technologies such as wind turbines and natural gas power plants. The numbers shown represent the total installed capacity of the technology in each zone.

of hydrogen. This means that hydrogen injection is maximised (20 vol.%) at times of low gas demand, but much lower at times of high gas demand, resulting in an average injection rate of around 10 vol.%. To achieve higher average levels of injection than 10 vol.%, additional infrastructure (in particular hydrogen storage) must be installed to provide more hydrogen supply flexibility. This increases costs, so that higher levels of FIT are required to make it worthwhile. With a FIT of £50/MWh, average hydrogen injection across the whole system exceeds 17 vol.%, and the majority of the network has been upgraded for hydrogen injection.

Details of the hydrogen system design in the case with a FIT of £50/MWh case are shown on the right of Figure 5-9. In this case, hydrogen is produced entirely by SMR with CCS. SMR plants are built in two locations, each with offshore CO_2 storage. A national hydrogen transmission system is established, connecting most of the country, and hydrogen is injected into the existing gas distribution system in all zones that are connected to this transmission system. With an established hydrogen infrastructure, hydrogen is also used to provide some flexibility to the electricity sector: hydrogen is extracted from storage at times of low electricity supply, and converted to electricity in fuel cell plants. Overall, 80% of hydrogen is injected into the gas distribution grid, 15% is used in fuel cells for power, and the remainder is used for other heating applications such as industrial use.

Finally, the effect of the grid upgrade cost assumptions for hydrogen injection can be seen in Figure 5-8. With upper bound cost estimates, a greater incentive for hydrogen injection is required (a FIT of approximately £10/MWh more is needed to achieve a similar level of hydrogen injection). However, lower bound upgrade cost assumptions have little influence on the overall level of hydrogen injection.

5.4.1.2 Cost of hydrogen and impact on consumer bills

Figure 5-10 shows the levelised cost of hydrogen in the gas grid for the scenario with a FIT of £20/MWh and the scenario with a FIT of £50/MWh. These costs represent the average cost of all hydrogen injected into the gas grid. This cost is not equal to the FIT, primarily because the "optimal" level of injection for a given FIT will be driven by the marginal cost of injection (rather than the average cost), but also because of other factors such as the profitability of alternatives, such as injection of natural gas.

The costs of grid upgrades contribute a relatively small amount to the overall cost of hydrogen in the gas grid. In both cases, less than 3% of the cost of hydrogen in the gas grid is attributed to gas grid upgrades (based on the central cost estimates). In the

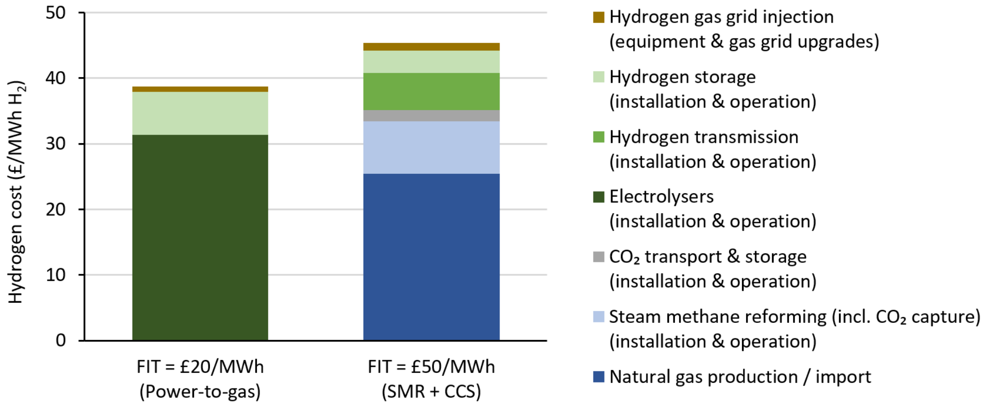


Figure 5-10: **Levelised cost of hydrogen injected into the gas distribution grid for hydrogen produced from power-to-gas and hydrogen produced from SMR (with CCS).** Costs shown are with baseline injection cost assumptions. The power-to-gas case is taken from the scenario with a feed-in tariff of £20/MWh, and the electricity price is not included. The SMR case is taken from the scenario with a feed-in tariff of £50/MWh.

£50/MWh case, in which hydrogen is produced from SMR, over half of the hydrogen cost is the cost of the natural gas feedstock. In the £20/MWh case, in which the hydrogen is produced from power-to-gas, electricity cost is not included in the levelised hydrogen cost. Most of the hydrogen in this scenario is produced overnight, from "excess" electricity which can be assumed to have a low or even zero cost. Although Figure 5-10 shows that the hydrogen from power-to-gas has a lower cost than hydrogen from SMR in these scenarios, only a limited amount of excess electricity is available for this power-to-gas. Larger scale power-to-gas would have to compete with other demands for electricity, therefore increasing the levelised hydrogen cost. Consequently SMR becomes the preferred (lowest cost) hydrogen production option as the scale of production increases.

These results suggest that partial hydrogen injection into gas grids is possible in present day energy systems and that hydrogen FITs in the range of £20-£50/MWh would help to establish hydrogen production and transmission infrastructures. Whilst no hydrogen FITs currently exist in the UK, FITs for biomethane injection are available in the range of £22-49/MWh [75]; Figure 5-8 suggests that a similar level of incentive for hydrogen injection would be sufficient.

The total annual costs of the FIT payments are £21m in the £20/MWh scenario and £1233m in the £50/MWh scenario. If these costs were to be funded by consumer gas bills, the average consumer's annual bill would increase by around £1 in the £20/MWh scenario and by £46 in the £50/MWh scenario[§]. Once these infrastructures are established, opportunities arise for hydrogen in other sectors, such as direct heating in specialist applications and providing flexibility to the electricity system by converting stored hydrogen to electricity at times of peak demand.

5.4.1.3 CO_2 impacts of partial hydrogen injection

The CO_2 emissions reductions resulting from partial hydrogen injection are small compared to the CO_2 emitted elsewhere in the system (predominantly in the combustion of natural gas for heating and electricity production). In the £20/MWh case presented above, hydrogen injection reduces gas distribution grid emissions by 0.1%, but this is offset by increased natural gas usage elsewhere. In the £50/MWh case, the overall reduction in emissions across the whole system compared to the case with no hydrogen injection is 2.3%. In the modelled scenarios, power-to-gas hydrogen should in theory offer greater emissions reductions because it is powered mostly by excess wind and therefore has a near-zero CO_2 footprint. Meanwhile SMR hydrogen has a footprint of around 50 kgCO_2/MWh, due to the uncaptured emissions and upstream natural gas production emissions. However, the availability of excess renewables for power-to-gas is small, so this hydrogen production route does not offer emissions reductions at any significant scale.

5.4.2 Outlook for hydrogen and gas grids in 2050

In order to assess the long-term potential for hydrogen in gas grids, the GB energy system in 2050 was considered, taking into account GHG emission reduction targets. Emissions reduction targets can be imposed in the VWM using a constraint on total allowable emissions. The effect of different emissions constraints on the scenario results is determined in section 5.4.2.1. Subsequently, in section 5.4.2.2, the role of hydrogen in these scenarios is considered in detail.

5.4.2.1 Long term decarbonisation and the effects of emissions reduction targets

The UK has recently committed to achieving net-zero GHG emissions by 2050 [77]. However, a major challenge for achieving a net-zero target is the "unavoidable" emissions associated with fossil fuels. For example, even for processes with CO_2 capture, the

[§]Based on an average consumer using 15,000 kWh of gas per year [76].

rate of CO_2 capture rarely exceeds 90% [78, 79]. In some cases, higher rates of capture can be achieved, but this comes with a significant energy penalty [46, 80]. Furthermore, there are emissions associated with the upstream production of fossil fuels that are hard to avoid: for example, natural gas production can have GHG emissions of around 0.013 tCO_2 (equivalent) per MWh of natural gas produced [81]. These emissions could be avoided if fossil fuels were removed from the energy system altogether, however this would be a major challenge for the present day fossil-based system, especially by 2050.

These "unavoidable" GHG emissions are likely to mean that a "net-zero" emissions target will require negative emissions technologies (NETs), environmental restoration such as afforestation, and/or international CO_2 trading. The contribution that these options could make in the future is uncertain: the Royal Society and Royal Academy of Engineering estimated a maximum technical potential in the UK in 2050 of 130 $MtCO_2$/yr, including 50 $MtCO_2$/yr from biomass energy CCS (BECCS) and 25 $MtCO_2$/yr from direct air CCS (DACCS) [82]. In the Net Zero scenario in the National Grid Future Energy Scenarios, BECCS contributes 37 $MtCO_2$/yr in 2050 [83], whilst Daggash et al. model contributions from BECCS of up to 51 $MtCO_2$/yr and DACCS of up to 19 $MtCO_2$/yr [84].

As the focus of this study is on whether and how to utilise hydrogen in natural gas networks and not on which particular NETs could or should be employed, the scenarios considered in the section do not include any negative emissions technologies. However, to evaluate when the use of NETs becomes beneficial, the CO_2 emissions targets are progressively made more stringent in each scenario until a final target of zero emissions is reached. The marginal costs of meeting each additional target are calculated and thus it can be seen at which point further investment in and modification of the natural gas/hydrogen networks is less economical than employing NETs, based on their typical costs per tonne of CO_2 abated.

Figure 5-11 shows results from these scenarios, including the overall system cost and technologies used for electricity, heat and hydrogen production in each scenario. The electricity mix remains similar in all low-carbon scenarios, relying mainly on nuclear and wind power, although total electricity production grows from 460 TWh/yr in the 40 $MtCO_2$/yr scenario (representative of an 80% reduction in emissions from 1990 for the sectors modelled) to 662 TWh/yr in the zero-carbon scenario.

The increase in electricity production shown in Figure 5-11(a) is to provide heating, which is increasingly switched from natural gas to electricity. Whereas natural gas is used for 82% of domestic heating in the scenario with unlimited emissions (cf. section 5.4.1), this is reduced in each of the lower carbon scenarios and by the 10 $MtCO_2$/yr scenario natural gas is no longer used for domestic heating. In this scenario, almost all domestic heating is provided by electric heat pumps, except for 1% of heating that is provided by hydrogen by converting a portion of the natural gas grid.

Hydrogen has a role in these scenarios, without any specific incentives such as feed-in tariffs. The main use for hydrogen in these scenarios is in industrial heating, although hydrogen usage reduces with increasing CO_2 stringency. This is due to the unavoidable emissions associated with SMR, which is the cheaper hydrogen production option. Although increased production of hydrogen from electrolysis counteracts this to some extent, overall hydrogen production still reduces. The reasons for the preference to electrify heat rather than use hydrogen are discussed in section 5.4.2.2.

The system becomes increasingly more expensive with lower CO_2 emissions limits and the marginal cost of emissions reductions increases as the "easiest" emissions are eliminated first. Whilst reducing the overall system emissions from 40 $MtCO_2$/yr to 20 $MtCO_2$/yr costs on average £138 /tCO_2, reducing emissions from 20 $MtCO_2$/yr to 10 $MtCO_2$/yr costs £158 /tCO_2, and from 10 $MtCO_2$/yr to 5 $MtCO_2$/yr costs £259 /tCO_2.

From the increasing costs of the scenarios with more stringent emissions reduction targets, there is likely to be an optimal level of emissions that would be mitigated at a lower cost through negative emissions options. Estimates for the costs of negative emissions options such as NETs exceed £100 /tCO_2, and often more than £200 /tCO_2 [82]. Therefore, from the above scenarios, applying an emissions limit between 5 $MtCO_2$/yr and 20 $MtCO_2$/yr would provide the most pragmatic energy system design, with the remaining emissions reductions being achieved more cost effectively through negative emissions options. A detailed assessment of the actual NETs required is beyond the scope of this paper, as the focus is on the usefulness of HIGG.

5.4.2.2 Hydrogen injection into the gas grid in 2050

As the scenarios in section 5.4.2.1 show, the main alternative to converting gas grids to hydrogen is electrification of heating. There are many advantages and disadvantages of each of these options; in this optimisation study, the choice is driven primarily by cost and emissions. In this section, these issues are discussed and optimisation scenarios are presented that explore them in detail.

The assumptions used in this study for the investment costs of either converting gas grids to hydrogen or electrification of heating are shown in Table 5.2. For electrification,

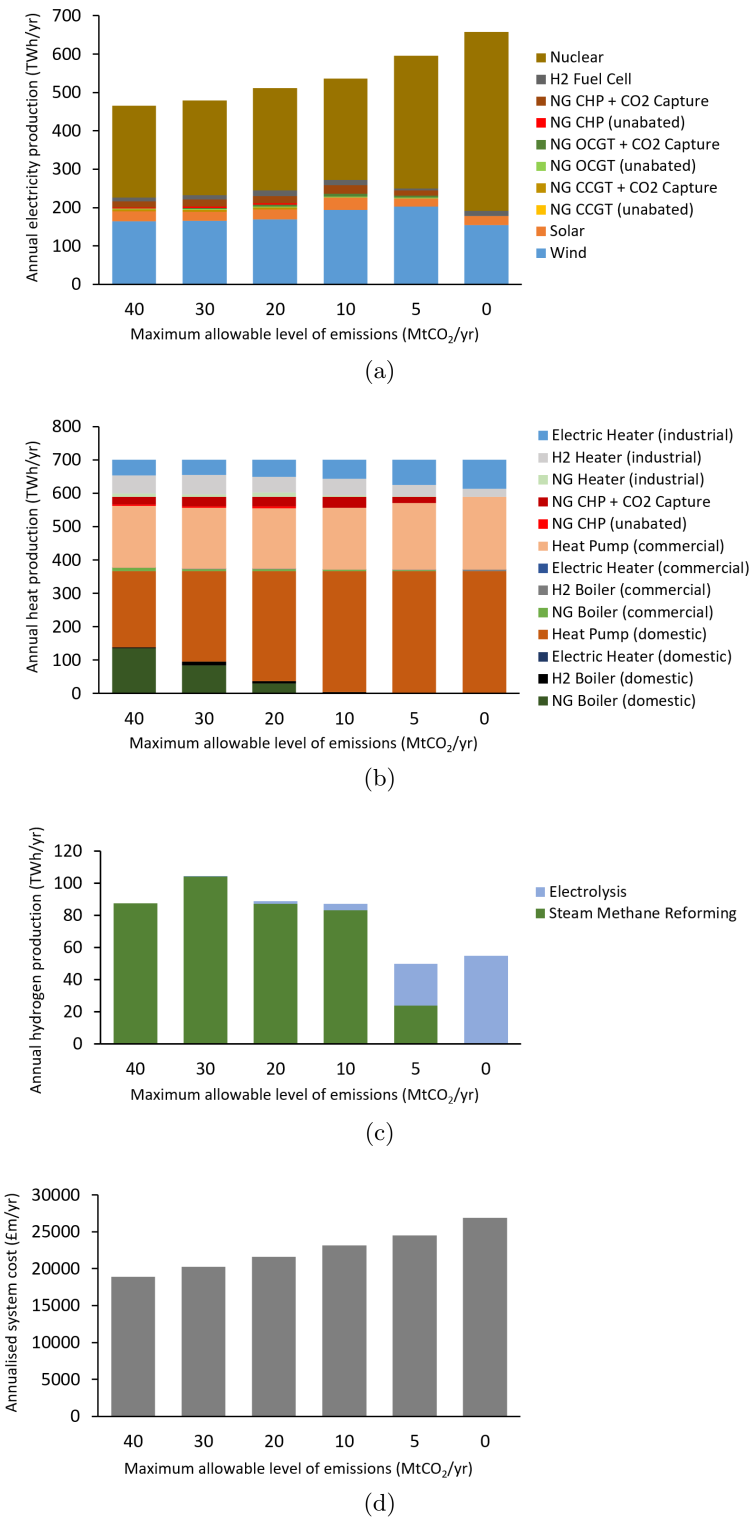


Figure 5-11: **Results from optimisation scenarios for 2050, with a range of allowable CO_2 emissions limits.** (a) Electricity production; (b) Heat production; (c) Hydrogen production; (d) Annualised overall system cost.

Table 5.2: Cost assumptions for investment in electrification of heating and conversion of gas grids to hydrogen. The central assumptions for 2050 are shown.

Electrification			Conversion of gas grids to hydrogen		
Investment	Cost	Ref.	Investment	Cost	Ref.
Expansion of electricity distribution infrastructure (cost per kW of new grid capacity)	£650	[64]	Conversion of existing gas distribution grids to hydrogen (cost per kW of grid converted)	£3.40	[46]
Installation of domestic heat pump and new heating system	£3,600	[65]	Installation of hydrogen boiler and heating system	£2,400	[55, 65]

it is likely that electricity distribution infrastructure would need expanding and that this would be more expensive than converting existing gas distribution grids to hydrogen. Meanwhile, given that the majority of homes currently have natural gas based heating systems, it is also likely to be more expensive to install electric heating systems (e.g. electric heat pumps, which typically also require new radiators [85]) than hydrogen systems (which would only require that the boiler be replaced).

However, although the investment costs for conversion of gas grids to hydrogen may be lower than electrification of heating, the hydrogen supply chain is more complex, relying on conversion of either natural gas or electricity to hydrogen. Electricity supply chains, however, are more direct between production of electricity and heating. Therefore the “fuel” costs are likely to be lower for electrification. Furthermore, the lower-cost hydrogen production route, via SMR, has unavoidable emissions associated with it, from the upstream natural gas production and the fraction of emissions that cannot be captured at the SMR plant.

The results in section 5.4.2.1 suggest that the lower supply chain costs of electrification outweigh the higher investment costs of upgrading/replacing the end-use technologies, when compared to conversion of gas grids to hydrogen. To explore this further, the significance of the cost assumptions in Table 5.2 were examined by modelling a series of scenarios with increasing electricity infrastructure costs. Scenarios in 2050 with investment costs between £650 per kW and £1250 per kW of new electricity distribution capacity were modelled, with emissions constraints of both 10 $MtCO_2$/yr and 20 $MtCO_2$/yr. No feed-in tariffs or other technology incentives were included in these scenarios.

The results from these scenarios are shown in Figure 5-12. Whilst with new electricity infrastructure costs at £650 per kW capacity there is almost no use of hydrogen in gas grids for heating, increasing electricity distribution costs make hydrogen more appealing and with costs of £1050 per kW capacity, with a CO_2 constraint of 20 $MtCO_2$/yr,

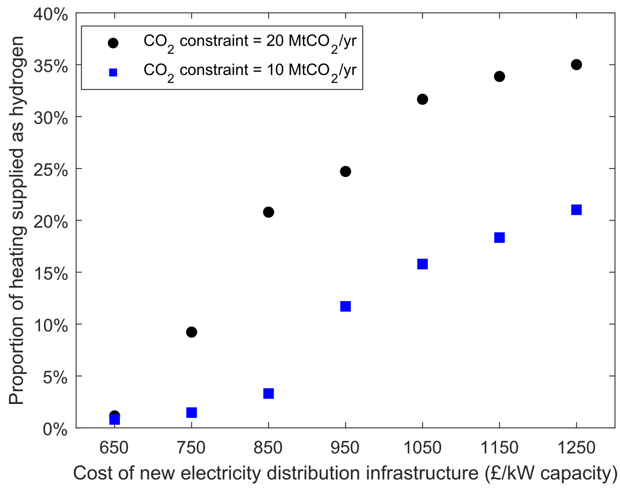


Figure 5-12: **Proportion of domestic and commercial heating supplied as hydrogen (through the gas grid) in scenarios with increasing costs of electricity distribution infrastructure.**

around one third of domestic and commercial heating is delivered as hydrogen through converted natural gas pipelines. A more stringent CO_2 constraint of 10 $MtCO_2$/yr results in less hydrogen being used due to the emissions associated with the hydrogen supply chain.

Figure 5-13 shows details of the system design and operation for the 20 $MtCO_2$/yr scenario with electricity distribution infrastructure costs of £1050 per kW capacity. An extensive hydrogen infrastructure is constructed, including hydrogen production from SMR, CCS, hydrogen and CO_2 transmission pipelines spanning the country, and a significant amount of hydrogen storage. The total annual hydrogen production is 291 TWh/yr, of which less than 1 TWh is from power-to-gas. A small amount (5%) of hydrogen is converted to electricity via fuel cells and the remainder is used for heating. As Figure 5-13(a) shows, different choices regarding conversion of natural gas distribution systems to hydrogen are made around the country. Overall, 57% of existing distribution grid capacity is converted to pure hydrogen, 26% is retained for delivering natural gas (including some partial hydrogen injection), and 17% is unused. Where gas grids are not used, electrification of heating is preferred.

Various hydrogen storage options are included to provide system flexibility. Underground storage facilities provide interseasonal storage for balancing variations in demand across the year, as shown in Figure 5-13(b). Linepack from the distribution and transmission systems provides some within-day flexibility but, importantly this is not sufficient for the whole system, so almost 300 GWh of pressure vessel hydrogen storage is also required. Typically the linepack and pressure vessel storage is accumulated overnight and depleted over the course of the day.

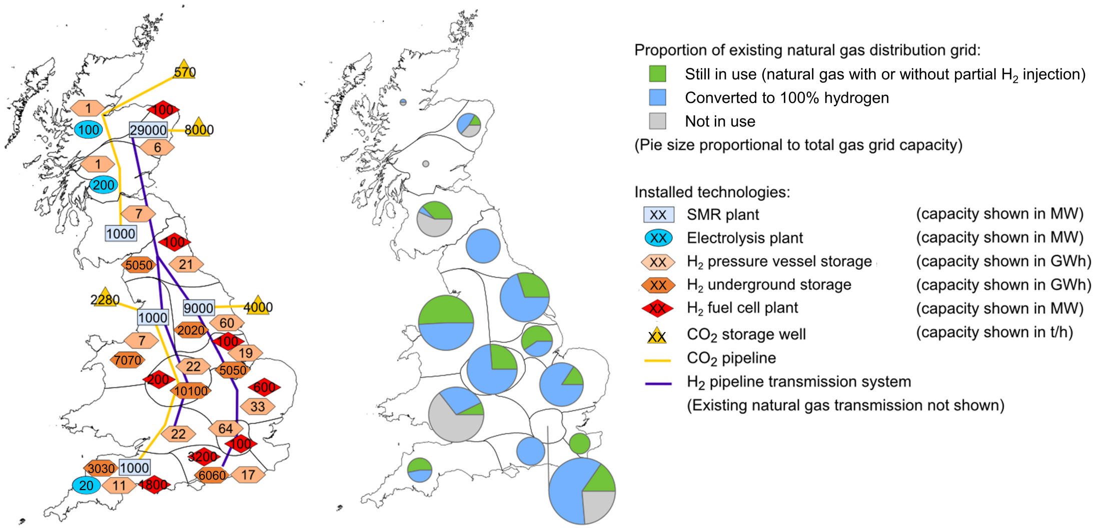
5.5 Conclusions

Hydrogen injection into gas grids, both through partial mixing with natural gas and complete conversion to hydrogen, is a feasible strategy for maintaining and decarbonising the extensive natural gas grids that serve many countries in the world. The advantages of hydrogen injection include reduced greenhouse gas emissions from the gas grid end users, making use of valuable transmission and distribution infrastructures (and avoiding expansion of electricity infrastructure), and exploiting the inherent flexibility that gas grids have, known as linepack flexibility.

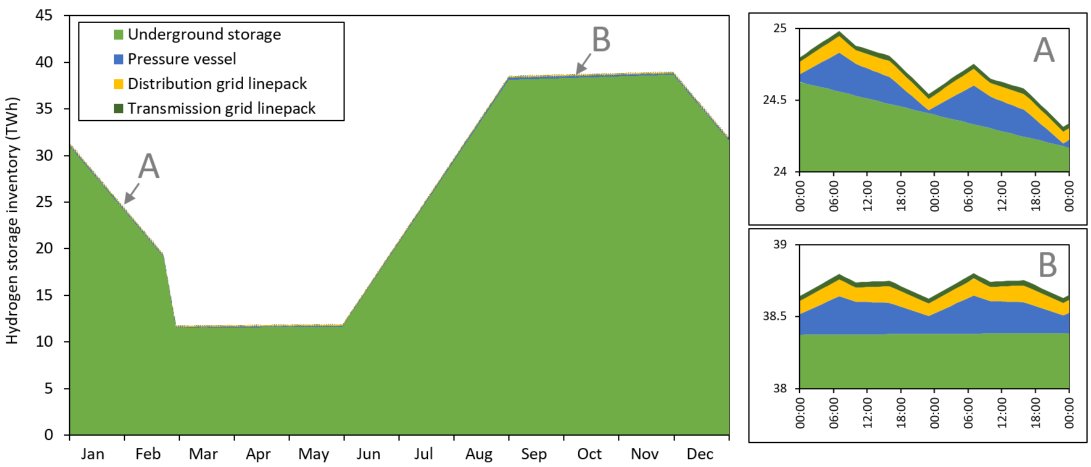
Although there are practical and safety challenges to utilising hydrogen in existing natural gas pipelines, most of these issues can be overcome or managed. Several testing and demonstration projects have been completed or are in progress globally that are expanding the knowledge base in this area and providing confidence on the feasibility of hydrogen injection.

Energy systems are ready for partial hydrogen injection into gas grids now. Using an integrated value chain optimisation model (the Value Web Model, which was further developed here to include hydrogen injection into the gas grid, conversion of gas grids to hydrogen, and linepack storage), this study has shown that feed-in tariffs of £20/MWh for hydrogen injected into gas grids would be sufficient to incentivise injection in certain applications. This would also provide some stability to the electricity system, by absorbing electricity at times of excess supply and converting to hydrogen using electrolysis. Higher feed-in tariffs, of around £50/MWh, would incentivise a wider roll-out of partial hydrogen injection, with average injection levels across the whole gas distribution grid in excess of 17 vol.%. In this scenario, an extensive national hydrogen infrastructure is developed, including hydrogen production from steam methane reforming and a national hydrogen transmission system. Partial hydrogen injection reduces gas grid emissions by up to 4 $MtCO_2$/yr, which is a reduction in overall system emissions of around 2.5%.

In the long term, complete conversion of gas grids to hydrogen is an option for decarbonising heat and exploiting the flexibility of gas grids. However, this option must compete with electrification of heat, which may have higher infrastructure costs but a more efficient energy supply chain. A particular challenge for conversion of gas grids



(a)



(b)

Figure 5-13: **Energy system design and operation for a 2050 case that includes conversion of gas grids to hydrogen.** The case shown is the case with a CO_2 constraint of 20 $MtCO_2$/yr and new electricity distribution grid installation costs of £1050/kW. (a) Maps of the energy system, including (left) installed hydrogen-related technologies (numbers show total installed capacity in the zone) and (right) proportion of the existing natural gas distribution grid that is retained, converted to hydrogen or unused in each zone; (b) Total storage inventory for all hydrogen storage options, including gas grid linepack, over the course of one year, with insets showing within-day variation in January and October.

to hydrogen in very low-carbon scenarios is the unavoidable CO_2 emissions from hydrogen production from fossil fuels. In this study, electrification of heating was found to be the optimal solution with median electricity infrastructure costs of £650 per kW capacity. However, conversion of gas grids could have a significant contribution if electricity infrastructure costs are found to exceed £1000 per kW capacity. Alternatively, other challenges for the electric heating supply chain, such as inadequate performance of electric heat pumps, would improve the case for conversion of gas grids to hydrogen.

Scenarios with significant proportions of the gas grid converted to hydrogen would involve an extensive roll-out of hydrogen-related infrastructure, including production plants, and transportation and storage infrastructure for both hydrogen and CO_2. Gas grid linepack would provide some flexibility to the system but this study found that the reduced linepack of gas networks when converted to hydrogen would mean that additional intra-day flexibility, such as above-ground hydrogen pressure vessels, may be required.

Provided that negative emissions options will be able to provide a small level of negative emissions (5-20 $MtCO_2$/yr for heating and electricity sectors considered in this study) a net zero emissions target is achievable and does not significantly affect the optimal 2050 energy system. However, achieving net zero emissions without negative emissions options would be significantly more expensive and would affect the final system design, primarily because this would preclude the use of any fossil fuels at all.

This study is the first to have applied value chain optimisation methods to hydrogen injection into gas grids, and the approach has provided valuable insights into the role of hydrogen and gas grids in the wider energy system. The model and insights presented here will be valuable to modellers and researchers looking to understand aspects of current and future energy systems, in particular the practicalities and the role of hydrogen injection into gas grids from a whole-system value chain optimisation perspective. The modelling scenarios in this paper have focussed on the energy system of Great Britain, as an example of a medium-sized energy system with an extensive natural gas grid. However, many other countries have a similar reliance on their gas grids, and the key insights from this study are applicable to these countries and the presented MILP formulation of the Value Web Model can be used together with country-specific data to obtain more direct results and insights. Finally, the results from this study will be valuable to policymakers, exploring the justification for incentives for hydrogen both now and into the future.

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Article appendices

The original Applied Energy article included appendices with abbreviations and the model nomenclature. In this thesis, the abbreviations can instead be found at the beginning of the article, and the full model nomenclature is provided in Appendix A of the thesis. The original article supplementary material, detailing the calculations performed for section 5.2.2, can be found in Appendix C of this thesis.

Chapter concluding remarks

The article that has been presented in this chapter provides valuable contributions to the thesis, including a study of key operational aspects of existing energy systems, and significant developments to the scenario modelling approach.

The article provides information on the design and operation of existing natural gas infrastructures, including linepack flexibility. Based on this, the opportunities and practicalities of injecting hydrogen into gas grids are discussed. In particular, the discussion in section 2.2 of the operational impacts of hydrogen injection on existing natural gas assets is valuable and timely, as there is significant interest in this area, and these impacts are not always considered. These practical issues were also used in the design of the scenarios that were modelled.

The most significant contribution of this chapter to the overall thesis is the additions to the scenario modelling approach. The various additions that were made in this chapter mean that the resulting scenarios provide a rich representation of hydrogen value chains within the context of a national energy system such as Great Britain. As has already been discussed in this thesis, the Value Web Model was already capable of many of the modelling requirements that were identified in Chapter 2 and Chapter 3, such as the combination of high spatial, temporal and technological detail with a wide system scope. The configurations made in this chapter add significant detail to the representation of hydrogen and associated value chains.

By including energy distribution networks, the value chains that deliver energy to consumers were represented in more detail. In particular, the costs of building and maintaining such networks were included, which is important as these costs could make a significant contribution to final energy costs. In the case of gas distribution grids, this also created the opportunity to model partial hydrogen injection, or conversion of the gas grid to hydrogen, including associated costs and impacts on operation. Finally, the mathematical formulation of the VWM was configured to enable the storage capacity of these distribution networks to be modelled, in addition to their delivery capacity.

Further modelling contributions in this chapter included modelling the linepack capacity of gas transmission systems, and expanding the model dataset. Solar power already makes a significant contribution to real-life energy systems, so its inclusion in the Value Web Model increases the model relevance and adds to the available value chains in optimisation scenarios. Similarly, inclusion of energy demands from the commercial and industrial sectors increases the scope of the model, and allows for a wider set of possible value chains, including opportunities for energy flows between sectors.

Beyond the methodological additions in this chapter, the scenarios considering the role of hydrogen injection within the Great Britain energy system also provide some interesting insights. Many of the trends in results from Chapter 4 were continued in this chapter. For example, cost optimal decarbonisation continued to focus on expansion of renewables rather than uptake of fossil fuels with CO_2 capture and storage. Nuclear power was also included in this chapter, and had a significant contribution to scenario results. Nonetheless, as expected, inclusion of industrial energy demands in this chapter resulted in a greater role for CO_2 capture than in Chapter 4, where only domestic demands were included. In the scenarios in this chapter, around half of industrial heat demands were satisfied by hydrogen produced from methane reforming with CO_2 capture, with the remaining demands satisfied by electricity.

With respect to hydrogen injection, in the near-term it was found that there are limited opportunities for partial hydrogen injection in existing markets, but a relatively low feed-in tariff would be sufficient to change this. Significantly, higher levels of hydrogen injection (e.g. greater than 10 vol.%) become increasingly expensive, due to the increased need for hydrogen production or storage infrastructure.

In the long-term, the scenarios in this chapter found that conversion of gas grids to hydrogen will have to compete with electrification of heat, which may prove to have a lower cost. The major challenge for conversion of gas grids to hydrogen is the cost of hydrogen production at scale. Whilst some hydrogen may be produced at low cost through power-to-gas, there is unlikely to be sufficient low-cost electricity for this production option to make a significant impact on gas grids. This finding continues the theme from Chapter 4, where it was found that the opportunities for hydrogen were focused on flexibility rather than bulk energy supply.

A further important insight from this study was the relatively small availability of linepack flexibility from gas grids that have been converted to hydrogen. This had previously been identified as a key advantage of converting gas grids to hydrogen, however, as was shown in section 2.2, the linepack flexibility of natural gas infrastructures is significantly reduced when converted to hydrogen. As a result, additional within-day hydrogen storage capacity is required in scenarios with conversion of gas grids to hydrogen, as discussed in section 5.4.2.2.

In this chapter, substantial developments to the scenario modelling methodology have been made, and scenarios have been presented that begin to explore the potential of hydrogen and gas grids in future low-carbon energy scenarios. In the following chapter, these scenarios will be expanded in order to further develop the findings of this chapter.

Two clarifications to the article presented in this chapter should be noted, which have been identified since it was published:

- It should be noted that Equation 5.2 is essentially the Poiseuille equation.
- In Figure 5-5, the meaning of spatial zones z and z' is not clear. These are two representative spatial zones, for example representing regions of a country. Each spatial zone can have its own resource availabilities (e.g. wind and solar) or demands (e.g. heat or electricity). As the diagram illustrates, each of the technologies included in the model can optionally be installed in a spatial zone (subject to any constraints, e.g. land use). Additionally, transportation technologies can be installed, to move resources between spatial zones. Two representative zones are shown in Figure 5-5, but any number of zones may be modelled in practice (16 spatial zones are used to represent GB in this thesis).

Chapter 6

How to incentivise hydrogen energy technologies for net zero: Whole-system value chain optimisation of policy scenarios

Chapter introductory remarks

This chapter is based on a research article that has been submitted to the Elsevier journal Sustainable Production and Consumption, and is currently under review. If accepted for publication, the copyright will rest with the publisher, but they permit re-use in theses, provided that the journal is referenced as the original source. The submitted article details are as follows:

> Christopher J. Quarton and Sheila Samsatli. How to incentivise hydrogen energy technologies for net zero: Whole-system value chain optimisation of policy scenarios. *Sustainable Production and Consumption* [Under Review].

This is the final "research" chapter of the thesis. The study presented in this chapter builds on the previous modelling chapters, primarily by exploring a new set of scenarios in detail.

In the scenarios in previous chapters, although hydrogen often arises in the optimisation results, it tends to have a relatively supplementary role, unless specific hydrogen incentives are included. Therefore the main objective of this study was to understand the impacts of different policy interventions on the uptake of hydrogen within the system. This also provides the opportunity to explore the roles of hydrogen and alternative value chains in more detail.

The article starts with a review of the different policies that are available to governments for supporting energy technologies. This review provides some clarity on the wide range of policy tools available, and also considers their applicability to hydrogen technologies. As the literature review in the article describes, whilst many previous reviews of energy policies have been performed, they typically focus on the effectiveness of past policies, rather than considering them in the context of emerging technologies. The review that is provided was also used to develop the scenarios for the modelling work of this article.

Building on the modelling work of previous chapters, the scenarios that are modelled in this study have the most complete representation of the energy system of any of the scenarios in this thesis. A significant addition to the scenarios in this study is the inclusion of a bioenergy value chain for producing hydrogen. It is acknowledged that bioenergy is a complex area that is mostly beyond the scope of this thesis. However with growing interest in bioenergy, especially for its potential to generate negative CO_2 emissions, it is important to include some consideration of bioenergy value chains for hydrogen production. Including bioenergy value chains with net negative CO_2 emissions also enabled the modelling of "net-zero" energy scenarios. Although a net-zero scenario was modelled in Chapter 5, no net negative CO_2 value chains were available, so all fossil fuels were excluded from the net-zero scenario results.

A further important aspect of the scenarios in this study is that they include an optimisation of four sequential decades at once, spanning from the present day to 2060. This was also the case in Chapter 4, but due to the larger model size in Chapter 5, only single decades were optimised (either in the present day, or 2050). In the study presented in this chapter, despite the increased computational demands, four decades were optimised in order to gain an understanding of the transition of the energy system between the present day and the net-zero system in 2050.

Following this introduction, an authorship declaration is provided, followed by the article as submitted to Sustainable Production and Consumption (although re-formatted for this thesis). The article includes its own reference list. The original article appendices are not presented in this chapter, but a guide to where the contents of the original appendices can be found is provided at the end of the article. Finally, some concluding remarks are provided at the end of the chapter, including further discussion of the contribution of the article, and its relevance to this thesis.

Authorship declaration

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How to incentivise hydrogen energy technologies for net zero: Whole-system value chain optimisation of policy scenarios</td></tr>
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<tr><td>Candidate's contribution to the paper</td><td colspan="3">The candidate contributed to / considerably contributed to / predominantly executed the...
Formulation of ideas:
70% - I formed the initial ideas for the study, which I then developed with help from S. Samsatli and feedback from presentations at BEIS and conferences.
Design of methodology:
70% - Building on the version of the Value Web Model from the last chapter, I configured the model and designed the scenarios that were modelled in this study, with support from S. Samsatli.
Experimental work:
95% - With some assistance from S. Samsatli, I assembled the model input data and carried out all of the model runs, post-processing and analysis.
Presentation of data in journal format:
80% - I structured and wrote the article, and designed all of the figures. S. Samsatli provided comments on the draft, made final edits to the manuscript for submission to the journal and helped address reviewers' comments.</td></tr>
<tr><td>Statement from candidate</td><td colspan="3">This paper reports on original research I conducted during the period of my Higher Degree by Research candidature.</td></tr>
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Article:

How to incentivise hydrogen energy technologies for net zero: Whole-system value chain optimisation of policy scenarios

Abstract

Policy intervention into energy systems will be essential if they are to meet decarbonisation targets. As shown by the examples of wind and solar power, policy support of emerging energy technologies can lead to long-term benefits to the energy system. Hydrogen technologies are emerging technologies that, with sufficient policy support, can provide valuable energy services. This study analyses the policies available for encouraging energy decarbonisation as well as supporting emerging energy technologies, and examines their implications for hydrogen technologies. The effectiveness of these policies is then assessed through value chain optimisation. Policies for ensuring that a system achieves net-zero emissions are modelled and it is found that both carbon budgets and carbon taxation can achieve this. The policy design, including decarbonisation trajectory, significantly influences the overall system costs and emissions. In a net-zero energy system, hydrogen has a role in industry without needing specific policy support. However, for further uptake of hydrogen, such as for injection into the gas grid, policy intervention is necessary. For decarbonising domestic and commercial heat, hydrogen is found to be more expensive than electrification, primarily due to the costs associated with producing hydrogen at scale. Both feed-in tariffs and obligations for hydrogen injection were found to be effective at increasing hydrogen uptake, although with an increase in overall system cost of £11--14 for each additional MWh of hydrogen.

Abbreviations: AIMMS: Advanced Interactive Multidimensional Modeling System; CCGT: Combined Cycle Gas Turbine; CCS: CO_2 Capture and Storage; CfD: Contracts for Difference; CHP; Combined Heat and Power; CO_2: Carbon dioxide; COP: Coefficient of Performance; CPF: Carbon Price Floor; ETS: Emissions Trading System; FIT: Feed in Tariff; GB: Great Britain; GHG: Greenhouse Gas; H_2: Hydrogen; ICE: Internal Combustion Engine; IEA: International Energy Agency; LCFS: Low Carbon Fuel Standard; OCGT: Open Cycle Gas Turbine; RHI: Renewable Heat Incentive; RO: Renewables Obligation; RPS: Renewable Portfolio Standard; RTFO: Renewable Transport Fuel Obligation; SMR: Steam Methane Reforming; tCO_2: Tonnes of Carbon dioxide; VWM: Value Web Model.

6.1 Introduction

Energy systems are likely to require new energy technologies and carriers, such as hydrogen, in order to decarbonise, but government intervention is likely to be necessary to help these technologies establish themselves. Well-designed government intervention requires an understanding of both the optimal pathway to decarbonisation and the efficacy of the policy options available. In this study, different policies for bringing about decarbonisation and supporting new energy technologies are considered and modelled through value chain optimisation, focussing in particular on the role of hydrogen.

6.1.1 Context

There is increasing consensus that energy systems will need to reach net-zero emissions in order to prevent the worst effects of climate change [1]. Whilst this may be technically possible, it will require government intervention to support low-carbon technologies and shift away from existing greenhouse gas (GHG) emitting technologies. However, it is important that the energy transition is both equitable and cost-effective, so the design of any government intervention must be considered carefully.

For energy systems to eliminate GHG emissions, various technology solutions will be needed, including both well-established technologies (such as wind turbines and solar PV) and emerging technologies. Hydrogen is one emerging solution that may have an important role in helping to decarbonise energy systems [2]. Hydrogen is an alternative energy carrier to electricity or fossil fuels, and can be converted to heat or electricity without generating GHG emissions. If hydrogen is produced via electrolysis (powered by renewable electricity), from bioenergy, or from fossil fuels with carbon capture and storage (CCS), then the production of hydrogen is also low-carbon. There are many possible applications for hydrogen, including heating in homes and industry; as a transport fuel; for bulk electricity storage; and as a chemical feedstock [3].

However, it is unclear exactly how hydrogen should be used to maximise its benefit to decarbonising energy systems, and key hydrogen technologies (e.g. electrolysers and fuel cells) are yet to mature sufficiently to make significant contributions to energy systems. Governments can support these technologies, and doing so now could save GHG emissions and costs in the long run. However, government intervention must be carefully designed to ensure that the energy transition is both cost-effective and equitable.

6.1.2 Literature review: modelling to evaluate energy policy options

Scenario modelling can be valuable for assessing the effectiveness of energy policies, by modelling scenarios in which different policies are imposed and measuring the consequences using metrics such as technology uptake, costs, and environmental impacts [4]. Chai and Zhang [5] used modelling to compare energy policies within the China energy system, emphasising that increased spending was needed throughout the research, development and demonstration stages for emerging energy technologies. Meanwhile, Martinsen [6] assessed the interactions between domestic policies and global learning rates on the uptake of new technologies in Norway, through MARKAL-based modelling, finding that domestic subsidies could encourage uptake of technologies, but have limited impact on emissions. Global energy scenario studies, such as the World Energy Outlook [7], also model energy policies but generally have little comparison of policy options. Often these studies use explorative scenarios, which focus on policies that are already in place or planned, and they can therefore underestimate the uptake of emerging technologies [4].

Whilst general policy studies are valuable, hydrogen has unique characteristics, so needs specialist consideration. Many energy policy studies focus on the electricity sector, and hydrogen can contribute here, but it could also span other sectors including heat, industry and transport. Furthermore, hydrogen is an energy carrier that has multiple technologies and infrastructures associated with it, such as electrolysers, fuel cells, hydrogen storage and hydrogen transportation infrastructures, therefore the challenge may be to establish multiple different technologies concurrently: a chicken-and-egg problem [8].

Various reviews have assessed the potential of hydrogen and provided recommendations for future policies. Ball and Weeda [8], for example, state the need for robust policy support of hydrogen, both in the level and longevity of the support provided. The Hydrogen Council argue that hydrogen can scale up and become cost competitive in many sectors, but only with significant support, including regulatory support, infrastructure investment, financial support and new market creation [9]. The IEA have argued that policies are needed to stimulate commercial demand for hydrogen, mitigate risks, and promote research and development [3].

Several studies have modelled hydrogen within energy systems but with little consideration of policies beyond decarbonisation constraints. Panos et al. [10] and Blanco et al. [11] both used TIMES-based models, of the Switzerland and EU energy systems respectively, to model hydrogen and other technologies under varying decarbonisation constraints. McPherson et al. [12] used MESSAGE to model electricity storage options (including hydrogen) in scenarios with and without a CO_2 tax, finding that increased levels of R&D for flexibility technologies were needed in scenarios without CO_2 taxes. Cerniauskas et al. [13] optimised hydrogen supply chains to compare the competitiveness of hydrogen with incumbent energy carriers under various CO_2 tax rates. In a roadmap study for hydrogen in the Flanders region of Belgium, Thomas et al. [14] modelled various hydrogen case studies, and made recommendations for future hydrogen policies, but did not model them.

Net-zero has only recently become an ambition for many energy systems, and is likely to affect hydrogen uptake, however it was not modelled in any of the studies mentioned above. Panos et al. [10] and Blanco et al. [11] both identified that more stringent decarbonisation constraints typically lead to a greater role for hydrogen in the scenario results. For many of the hardest-to-eliminate emissions, for example in industry or long-haul transport, hydrogen is the low-carbon alternative with the most potential [15]. Therefore, moving to an ambition of net-zero emissions is most likely to increase the demand for hydrogen, so this should be accounted for in modelling studies.

Some studies have modelled hydrogen-specific incentives but all have focussed on Feed-In Tariffs (FITs). Scamman et al. [16] modelled a range of business case studies for power-to-hydrogen and injection into the gas grid with varying FITs, capital grants and electricity prices, finding that with appropriate support now, learning rates would make power-to-gas self-sustaining by 2030. Budny et al. [17] also modelled some business case studies, focussing on storage and access to balancing markets in Germany, but found that high FITs were necessary to achieve profitability. Finally, Quarton and Samsatli [18] assessed the prospects of hydrogen injection into the gas grid in the UK through value chain optimisation, finding FITs of £20/MWh to be sufficient to incentivise low levels of partial injection in the present-day system.

6.1.3 Contributions and structure of this paper

This study provides the first analysis of policy incentives for hydrogen, and considers hydrogen technologies within the electricity, heat and industrial sectors. A range of policies are evaluated, including capital grants, hydrogen feed-in tariffs, and obligations on hydrogen uptake. Additionally, different CO_2 taxation and CO_2 budget policy strategies are evaluated. The assessment includes value chain optimisation of a national energy system, with the goal of reaching net-zero emissions by 2050. This approach enables the optimisation of both the design and operating strategy for various energy value chains. Optimal value chains can then be compared, accounting for efficiencies, costs, environmental impacts, and interactions with the wider energy system. A detailed spatio-temporal representation is used, with multiple spatial zones and representation of energy system dynamics at different temporal scales, including hourly, seasonal and decadal. This study represents the first time that value chain optimisation has been used to evaluate and compare the effectiveness of different policy interventions, providing a holistic analysis of the different pathways to net-zero and comparing them in their optimal configurations.

Section 6.2 discusses the available policies for encouraging an energy transition. The scenario modelling method is then described in Section 6.3, including details of the Value Web Model used for the value chain optimisation, and details of the scenarios that were modelled. Section 6.4 presents and discusses the results of these scenarios, and finally conclusions are given in Section 6.5.

6.2 Policies to incentivise energy technologies

This section examines the policy tools available to governments for encouraging energy transitions. Figure 6-1 presents an overview of the policy types considered in this section, including the stage of technology development at which they are typically used. Policies are separated into two categories: policies for penalising existing technologies and policies for supporting emerging technologies. More details on these policies, including actual examples and discussion of how they may be applied to hydrogen, are given in the following subsections.

6.2.1 Penalising existing technologies

A key challenge for energy policy is to correct for energy market failures, such as negative externalities [19]. For example, well-established, low-cost technologies often have adverse environmental impacts which can be penalised by policy intervention. This may either encourage these technologies to innovate (e.g to reduce CO_2 emissions), or create a more level playing field for emerging technologies.

Table 6.1 summarises the policy types that are considered in this section, with some real-life examples. Typically these policies are used to penalise well-developed technologies, but could also be used for less-developed technologies.

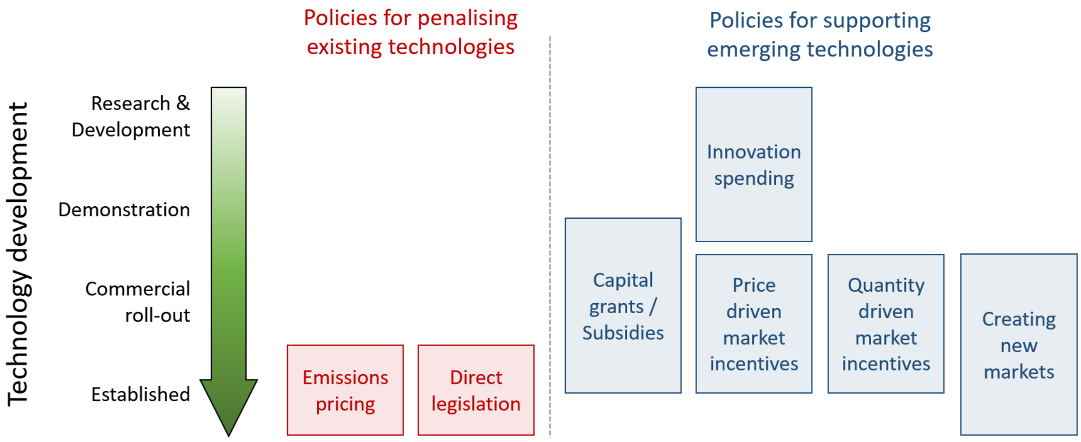

Figure 6-1: **Policy options for either penalising existing energy technologies or supporting emerging technologies.** The vertical positions of the policy types indicate the stage of technology development at which they are typically applied.

Table 6.1: Categorisation and examples of policies aimed at penalising existing energy technologies

Category	Examples			
	Location	Policy	Sector	Ref.
Emissions pricing				
Carbon tax	British Columbia	Carbon tax	All *	[20]
Carbon cap and trade	EU	Emissions Trading System (ETS)	Industry, Electricity	[21]
Direct legislation				
	Various	Vehicles emission standards	Transport	[22]
	Various	Ban on sales of vehicles with internal-combustion engines	Transport	[23]
	UK	Coal & wet wood ban (Clean Air Strategy)	Heat	[24]

* Greenhouse gas emissions from all combustion of fossil fuels are included, excluding a few minor exemptions [20].

6.2.1.1 Emissions pricing

Emissions pricing is widely discussed for incentivising emissions reductions, and there are some examples of successful emissions pricing policies. A detailed discussion of the wider economic merits and drawbacks of emissions pricing is beyond the scope of this study but many valuable reviews have been written on the subject (e.g. [21, 25, 26, 27]). This section describes the main options for emissions pricing and discusses how they might influence emerging energy technologies, in particular hydrogen.

Emissions pricing aims to account for the negative externality that is GHG emissions by imposing an additional cost on emitters [26]. Whilst this does not directly influence emerging technologies, it makes incumbent, high-emission technologies more expensive, which may allow low-carbon alternatives to enter the market, or encourage emitters to invest in decarbonisation. Two common approaches for emissions pricing are carbon taxation or carbon cap-and-trade.

With a carbon tax, governments collect tax for each tonne of CO_2 emitted by each organisation within the taxation system [25]. Carbon taxes are relatively straightforward to implement and generate a revenue stream for the government, but they are also a relatively blunt tool and could be regressive if the collected revenue is not re-distributed equitably [27].

In British Columbia a carbon tax has been implemented relatively successfully: in 2015, Murray and Rivers [20] estimated that the tax had helped to reduce emissions by between 5% and 15%, with negligible impacts on the wider economy. The scheme was designed to be revenue-neutral, with tax revenues being redistributed through various fiscal measures, to limit the social impacts. Carbon taxes have also been introduced in Sweden, New Zealand, and Chile [27].

Carbon cap-and-trade (also known as carbon trading or emissions trading) is an alternative to carbon taxation, where an allowable level of emissions across the whole system is determined, and emissions allowances are allocated to all organisations within the system [21]. Allowances can be traded so that emitters can either reduce their own emissions or purchase allowances from others. The total number of allowances can be reduced over time, reducing overall emissions. An advantage of carbon-trading schemes is that the market determines the most cost-effective way to eliminate emissions, with the price of emissions allowances (CO_2 trading price) being influenced by the rate at which decarbonisation is achieved. However, the scheme must be carefully managed to ensure that the CO_2 trading price is sufficiently high and to prevent emissions leakage into other countries outside the scheme [26].

Examples of carbon-trading schemes include the EU Emissions Trading System (ETS), and schemes in Switzerland, South Korea, California, and China [21]. Early carbon-trading implementations faced some operational issues, such as overestimation of allowable emissions, but more recent implementations (e.g. in California and South Korea) have learned lessons from these issues and been designed more carefully [21].

In some cases, carbon taxes are used in combination with carbon-trading schemes, to cover aspects not accounted for by the trading scheme. In the UK, for example, the Carbon Price Floor (CPF) sets a minimum limit for the CO_2 trading price. If the price falls below the CPF, the price difference is collected as tax [28]. In France, a carbon tax is imposed on emissions that fall outside of the EU cap-and-trade scheme, such as transport and domestic heating [20].

6.2.1.2 Legislation

Direct legislation can be used to specify standards for technologies (e.g. allowable emissions levels), or whether certain technologies are allowed to operate at all (e.g. banning the worst-polluting technologies). In the transport sector, many governments have requirements for allowable levels of emissions for vehicles [22], and several governments have announced plans to ban the sales of internal-combustion engine (ICE) vehicles altogether [23]. Similar measures exist in other sectors: in the UK, for example, the sale of coal and wet wood for use in domestic heating has been banned on air-quality grounds [24].

These policies could influence hydrogen technologies. Hydrogen fuel cell vehicles are an alternative to ICE vehicles, for example, so they are likely to benefit from the ban on ICE vehicles. Similar effects would be achieved in other sectors: in the heat sector, for example, low-carbon technologies would benefit if natural-gas boilers were banned.

A challenge for policies intended to penalise existing technologies, whether through emissions pricing or direct legislation, is vested interests. Penalised technologies are likely to have stakeholders who stand to lose if these technologies are made less competitive or banned altogether, and these stakeholders may attempt to influence legislation to reduce its potency. Consequently, policies in this category may require a strong mandate for the government to overcome these vested interests.

Table 6.2: Categorisation and examples of policies for supporting emerging energy technologies

Category	Examples			
	Location	Policy	Sector/Application	Ref.
Technology development				
Innovation spending	USA	DOE Hydrogen and Fuel Cells program	Various	[29]
	Japan	Basic Hydrogen Strategy	Various	[30]
	EU	Fuel Cells and Hydrogen Joint Technology Initiative	Various	[31]
Technology roll-out				
Capital grant/subsidy	Various	Support for wind and solar installations	Renewable electricity	[32]
	UK	Hydrogen for Transport Programme	Hydrogen refuelling	[33]
	California	Alternative and Renewable Fuel and Vehicle Technology Program	Hydrogen refuelling	[34]
Technology competitiveness				
Price-driven	Germany	Feed-in tariff (FIT)	Renewable electricity	[35]
	UK	Contracts for Difference (CfD)	Low-carbon electricity	[36]
	UK	Renewable Heat Incentive (RHI)	Heat / Gas	[37]
Quantity-driven	UK	Renewables Obligation (RO)	Renewable electricity	[38]
	UK	Renewable Transport Fuel Obligation (RTFO)	Transport fuel	[39]
	California	Low Carbon Fuel Standard (LCFS)	Transport fuel	[40]
New markets	Various*	Balancing markets	Electricity	[41]

* For example, the majority of EU countries have their own balancing markets, each with unique regulations [41].

6.2.2 Supporting emerging technologies

Support for new energy technologies can be provided throughout the technology life-cycle, including: technology development and demonstration; commercial roll-out; and aiding the technology's market competitiveness. Supporting new technologies may help them develop and become competitive in their own right, or correct for market externalities. The policy categories considered in this section, along with examples, are given in Table 6.2.

6.2.2.1 Supporting technology development

Government investment in technology innovation is important to help new technologies to develop, and should be provided to support the research, development and demonstration stages of the technology. The private sector may also invest in innovation, voluntarily or under government obligation, depending on the specific technology and present market need. Investment in innovation can help to develop prototypes, scale-up to demonstration and later commercial scale, improve performance, and reduce costs.

Most developed countries have energy innovation programmes, many including hydrogen. In 2018, International Energy Agency (IEA) member states spent €15.4 billion on energy research, development and demonstration projects, of which €478 million was spent on hydrogen and fuel cell projects [42]. Figure 6-2 shows historic innovation spending on hydrogen and fuel cells in IEA countries. Notable programmes include the US Department of Energy's Hydrogen and Fuel Cells programme, including the H2@Scale project [43, 44], various schemes as part of Japan's "Basic Hydrogen Strategy" [30], and the Fuel Cells and Hydrogen Joint Technology Initiative, part of the EU Horizon 2020 Framework [31].

For the energy transition, continued innovation spending will be valuable to hydrogen technologies at various stages of development. Many hydrogen technologies have been shown to be technically viable, but need further development and demonstration to prove functionality, scale-up, and achieve efficiency and cost improvements: example technologies include large-scale electrolysis and fuel cells, hydrogen gas turbines, hydrogen storage, hydrogen injection into gas grids, and use in long-haul and heavy duty transport [3]. Meanwhile there may be other technologies at earlier stages of development that have the potential for significant future contributions [45].

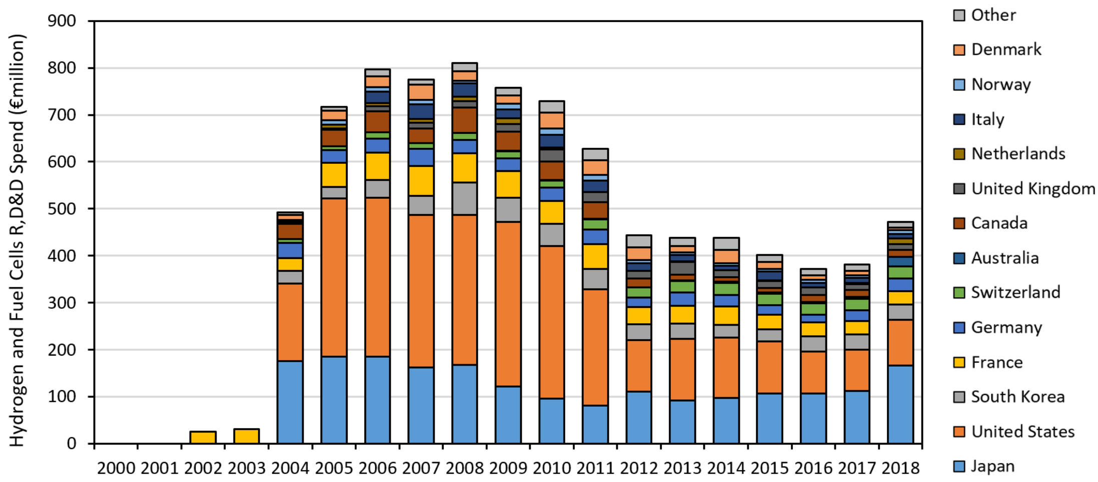

Figure 6-2: **Historic research, development and demonstration spending on hydrogen and fuel cells in IEA countries.** Data from [42].

6.2.2.2 Supporting technology roll-out

Capital grants or direct spending on a technology can be used to cover some or all of the upfront costs of installation: to encourage technology learning, or simply to aid roll-out of the technology so that it can provide system benefits (e.g. lower emissions) [32]. Capital grants and similar financial support have been used in numerous countries to support renewable-energy technologies; early examples include subsidies for wind turbines in the USA and Europe in the 1980s [46] and for solar PV in Japan in the 1990s [47].

This type of scheme already exists for hydrogen vehicle refuelling stations, including schemes in the UK [33], California [34], and Germany [48]. This approach is valuable because hydrogen vehicles rely on a well-established refuelling infrastructure: by helping to install the infrastructure, the purchase of hydrogen vehicles will be encouraged. Alternatively, grants for the purchase of the vehicle itself can be offered: such schemes already exist in the UK [49], Germany [50], California [51], Japan [52], South Korea [53], and China [54].

As with hydrogen for transport, hydrogen for heating relies on a hydrogen distribution infrastructure, so investment support for new hydrogen distribution infrastructure, or conversion of existing natural gas infrastructure to hydrogen, would reduce the obstacles to uptake of hydrogen for heating. Governments could also support the up-front cost of converting homes to hydrogen (e.g. new hydrogen boilers).

6.2.2.3 Supporting technology competitiveness

Whilst early support of technology development is necessary, support within markets may also be needed for technologies to establish themselves [19]. Penalising existing technologies can assist this by creating a more level playing field for emerging technologies, but is unable to target specific emerging technologies, so more developed (i.e. lower cost) technologies may be favoured. Therefore more direct support of emerging technologies through intervention into existing markets may be preferred: for example with price-driven incentives (adjusting market prices) or quantity-driven incentives (imposing requirements on the quantities of energy supplied by certain technologies). Alternatively, new markets can be created that aim to reward specific technology offerings.

Price-driven incentives

Feed-in tariffs (FITs) are a type of price-driven incentive that have widely been used in electricity markets to incentivise renewable generators, usually by guaranteeing a certain price for the renewable electricity. A prominent example of a FIT scheme was implemented in Germany to incentivise wind, solar PV, and biomass electricity generation by obliging electricity utilities to buy all generation from qualifying renewable generators at a pre-determined price [35, 55]. Different price-driven incentives have been used worldwide with different formats but performing similar functions. For example the contract for difference (CfD) scheme in the UK involves long term contracts with generators for a fixed price (the "strike" price). When the market price is below the strike price, the government pays the difference, but if the market price exceeds the strike price, the generator must pay the difference back [36].

Price-driven schemes also exist beyond the electricity sector. Under the Renewable Heat Incentive (RHI) in the UK, the government pays an incentive of around £22-49 for each MWh of biomethane injected into the natural gas grid [37, 56], and similar schemes exist in other EU countries [57]. Price-driven incentives can also support the energy consumer instead of the energy producer, for example making payments for each unit of heat generated by qualifying heating technologies [37].

A challenge for price-driven incentives is determining the incentive level. In the original German FIT scheme, the same fixed price was used for all qualifying generators, but this may enable projects with costs lower than this fixed price to capture surplus profit, whilst higher cost (e.g. less developed) projects may still struggle to compete [38, 58]. Therefore a technology-specific tariff may be preferred, as was later adopted in Germany [55]. Alternatively, auctions can be used to determine tariffs: in the UK CfD scheme, qualifying renewable generators bid with the rate they would receive for their electricity generation, and contracts are awarded to the lowest bids [36]. In this way, generator surplus profit should in theory be reduced [35]. This scheme also includes separate technology pots, so that less developed technologies do not compete with more developed technologies [36].

Although no examples of price-driven hydrogen incentives for producers are currently in use, similar models to those described above would be feasible for hydrogen. For example, studies have considered FITs for hydrogen injection into gas grids (e.g. [4, 16]), which could resemble the biomethane injection tariffs described above. Other price-driven hydrogen incentives are less obvious, as hydrogen is a separate energy carrier, so does not compete directly with existing energy carriers. The European Commission is considering a price-driven incentive to support low-carbon hydrogen in industry, using a contract-for-difference approach, linked to the carbon price [59]. Alternatively, payments could be made for the production of fuels synthesised from low-carbon hydrogen, such as synthetic methane, methanol, or Fischer-Tropsch hydrocarbons [60]. On the consumer side, price incentives could reduce the retail price of hydrogen as it competes with alternatives, for example transport fuels.

Quantity-driven incentives

Quantity-driven incentives, also known as Renewable Portfolio Standards (RPS), typically compel the market to purchase a quantity of the supported resource, allowing the market to determine the most cost-effective way of doing so [58]. Such schemes are often used in conjunction with tradeable certificates,, which can be traded between generators who have not reached their quota and those who have (and hence have surplus certificates). There may also be the option for generators to buy-out if they have missed the quota, by paying a pre-defined penalty price.

RPS schemes have been used in the electricity sector in various countries, including the UK, Italy, Australia and China [38, 61], but can also be used in other sectors. For example, as part of the Renewable Transport Fuel Obligation in the UK, large-scale suppliers of transport fuel must show that a percentage of the fuel they supply has come from renewable and sustainable sources, and tradeable certificates are used [39]. The Zero Emission Vehicle mandate, in use in 11 states in the USA, works on a similar principle, mandating that vehicle manufacturers supply a certain proportion of low emission vehicles, with a tradeable credit system [62].

Alternatively, quantity-driven schemes can specify a different parameter to control, such as CO_2 intensity. In California, for example, the Low Carbon Fuel Standard (LCFS) ensures that suppliers of transport fuel have a maximum allowable CO_2 intensity across all of the fuel they supply: credits are available for fuels with lower CO_2 intensities (and are also issued for electric and hydrogen charging and refuelling infrastructure), and can be traded to offset fuels with higher CO_2 intensities [40]. A CO_2 intensity scheme may not achieve the same results as a conventional RPS scheme: for example, a conventional RPS may not distinguish between wind and solar electricity generation, despite the two technologies having different levels of embedded CO_2.

Whereas price-driven incentives determine the level of incentive in advance, quantity-driven incentives can allow markets to determine how the quota is met, and the value of the qualifying generation (e.g. the trading price of certificates) [58]. This should minimise producer surplus profit, provided the certificate trading price settles at the marginal cost of production from qualifying sources. However, as with price-driven incentives, this may not be effective if some qualifying technologies have lower costs than others (e.g. because they are more developed) [38], so may need to be managed with separate technology categories (with separate certificates and quotas).

Accountability is important with quantity-driven schemes, as there have been instances where the quotas have never been met, either due to no enforceability (e.g. in China [61]) or a low buy-out penalty price (e.g. the UK Rewnewables Obligation [38]). Quantity-driven schemes may also present more investment risk, for example if the certificate market is unstable, which could increase overall costs. Finally, Haas et al. [38] suggest that quantity-driven incentives with certificate schemes may be more administratively complex and therefore more costly to implement.

As with price-driven incentives, quantity-driven incentives are most easily applicable to hydrogen in markets where it can compete directly with alternatives. For example in transport, hydrogen is already included within the LCFS used in California and elsewhere. Quantity-driven incentives could be implemented in gas markets if an obligation were imposed on gas suppliers to inject a minimum amount of hydrogen into their gas grids. Tradeable certificates could also be used, with different values depending on the CO_2 intensity of the injected hydrogen. Alternatively, a CO_2-intensity based scheme could be used, where gas suppliers are required to achieve an average CO_2 intensity for all injected gas; this approach would support both hydrogen and biomethane injection. Applications of quantity-driven incentives to support hydrogen in other sectors are less obvious but may be more achievable than price-driven incentives; examples could include an obligation for industries to switch to hydrogen where possible (e.g. in steel production and refining [3]), or a minimum required level of renewable hydrogen in industries that currently use fossil hydrogen.

In theory, quantity-driven incentives, especially those using tradeable certificates, may achieve lower system costs than price-driven incentives, as they encourage more competition between supported technologies. However, examinations of various EU schemes for supporting renewable electricity suggest that price-driven incentives have achieved greater technology uptake at lower cost [35, 38]. This may be due to the greater stability and lower regulatory and market risks of price-driven incentives, and may explain why some countries that initially adopted quantity-driven incentives, such as the UK and Italy, have more recently moved to price-driven systems. For either price-driven or quantity-driven incentives, technology-specific schemes are seen to be more cost effective than technology-neutral ones, as they help to minimise the surplus profit for the operators of lower cost technologies [58].

Creating new markets

If emerging technologies are unable to compete with incumbent technologies within existing markets, new markets can be created that value different characteristics. For hydrogen, markets that reward flexibility may be valuable. Flexibility is becoming increasingly important as intermittent renewables contribute more to energy systems, but conventional energy markets do not necessarily value this, instead focussing on a fixed price per unit of energy delivered [63]. Energy storage and transportation technologies, including hydrogen, could provide valuable services to energy systems but need markets to recognise this value.

Flexibility is most valuable in the electricity sector, due to the increasing penetration of intermittent renewables and the need for supplies and demands to be balanced instantaneously; in other sectors there are often already flexibility solutions in place, such as gas grid linepack flexibility [4]. Electricity flexibility is needed for a range of functions, including security of supply through backup capacity, rapid power ramping, supplying peak energy demands, and managing power quality [64]; markets must be found that value these services. In many countries the electricity transmission system operator already offers payments for flexibility services [41]. Typically, services are categorised based on response speed, ramp rate and response duration; payments may be a fixed payment per MW of capacity, per hour that the service is available, in addition to a payment for each MWh of energy used. Procurement of these services varies: in the UK, suppliers are selected from bids based on cost and the nature of the service being offered [65]. Localised flexibility markets are also begin to develop, via distribution network operators or independent platforms, that could enable small producers and even consumers to provide flexibility to the grid [66].

Hydrogen technologies could access these flexibility markets in various ways. Hydrogen is relatively easy to store, so could be used in dispatchable hydrogen turbines or fuel cells to provide rapid response [67]. Furthermore, hydrogen technologies can also be used for frequency control, either through turbines as synchronous generators, or with PEM fuel cells and electrolysers [68]. Power-to-gas with injection into the gas grid can link the electricity system to the gas system, creating opportunities to exploit the flexibility of the gas grid for electricity grid services [4].

Another example of new markets for hydrogen is in the chemicals and industrial sectors. Globally, around 33% of hydrogen usage is in refining, 27% is used for ammonia, and 10% is used for methanol, but more than 99% of this hydrogen is produced from fossil fuels, and the supply chains are not typically viewed as part of the energy system [3]. There could be opportunities for greater sector-coupling, with hydrogen for chemical and industrial uses being supplied from the energy system, for example from power-to-gas.

6.3 Methodology

The aim of this study was to examine the role of hydrogen throughout a transition from the present day to a net-zero energy system in 2050, applying a variety of decarbonisation and hydrogen-focussed policies. This was done by modelling different policy scenarios using value chain optimisation and comparing the optimal energy system configuration under each policy. The value chain optimisation methodology and details of the modelled energy system are given in Section 6.3.1. The design of the different policy scenarios, along with how they are modelled, is discussed in Section 6.3.2. Section 6.3.3 describes the computational statistics of the optimisation model. Finally, Section 6.3.4 provides a description of how the optimisation results were analysed to obtain important metrics and insights.

6.3.1 Energy value chain optimisation

The scenario modelling was performed using the Value Web Model (VWM), which is a mixed integer linear programming optimisation model for designing, and determining the operation of, integrated multi-vector energy networks. The mathematical formulation was developed by Samsatli and Samsatli [69, 70] and has recently been applied to develop low-carbon scenarios for: interseasonal storage and renewable hydrogen for heat [71]; hydrogen and carbon capture, storage and utilisation [72]; and gas grid linepack, power-to-gas and hydrogen injection into gas grids [18].

The VWM can simultaneously determine both the design of energy value chains and how they should be operated in order to maximise or minimise a particular criterion, or objective function, such as minimising system costs, minimising emissions or maximising net present value. Optimisation decisions include which energy resources should be utilised and when, which energy technologies should be installed, where and when, and how they should be operated. The VWM is a spatio-temporal model, meaning that it can account for the spatial distribution and temporal variation of a number of properties. These include: resource availabilities and energy demands that vary in both space and time, decisions about where to locate new technologies and when to invest in them (i.e. long term energy system planning over multiple decades) as well as how to operate them on a seasonal, day-to-day and hourly basis. The spatial and temporal representation of the model allows it to include a detailed account of energy storage and transportation/transmission of resources.

This approach to modelling energy systems is valuable, as it is able to represent large-scale details, such as the overall decarbonisation pathway and system costs, whilst also representing detailed aspects of the energy system (which affect the overall performance of the system). For example, specific results such as how a single technology is operated over the course of a day can be examined. Different modelling constraints can be imposed to represent policy interventions on the system, for example controlling CO_2 or subsidising particular technologies. Hence the effects of these policy interventions on the system design, operation, costs, and environmental impacts can be assessed.

The VWM can represent a wide range of energy resources (e.g. electricity, hydrogen and natural gas) and technologies (e.g. conversion technologies, storage technologies and transmission technologies). Figure 6-3 shows a schematic of the resources and technologies that are included in the scenario studies and how they are interconnected.

In general, there are three different types of resource that can be modelled in the VWM. Primary resources, such as wind or natural gas, have limited availabilities (e.g. dependent on wind speed profiles and land area) and can be extracted for use in the energy system. Some primary resources, such as wind and solar, require "resource utilisation" technologies (wind turbines and solar PV) to extract and use the available energy. Some resources represent final energy services, such as electricity and heat, and have spatio-temporal demands that must be satisfied. Finally, the other resources represent intermediates or wastes, such as some energy carriers and CO_2 (which can be

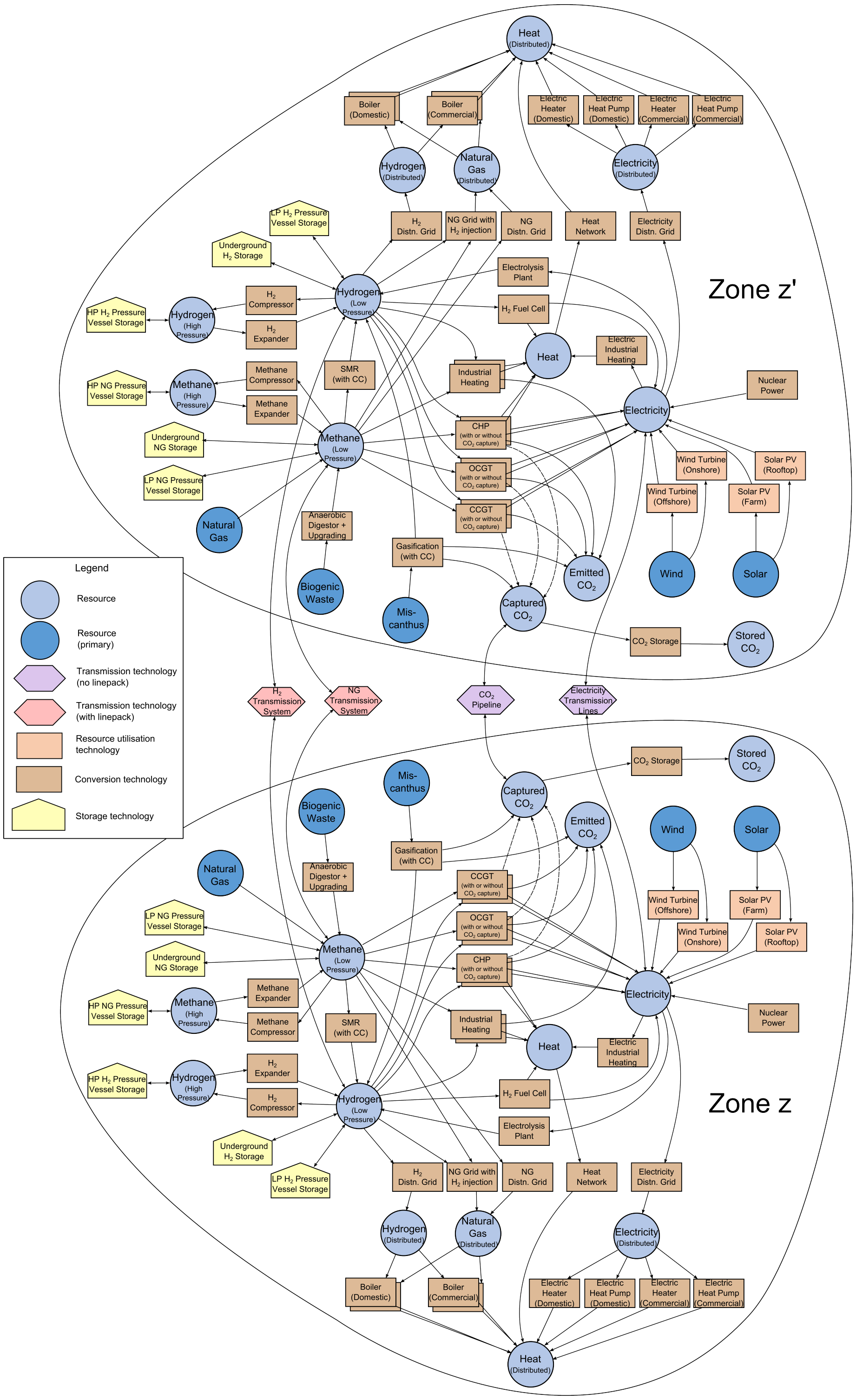

Figure 6-3: **Diagram showing the resources and technologies considered in this study.** Primary resources are available that may be converted by conversion technologies to eventually produce resources that satisfy energy demands. Two spatial zones z and z' are shown: transportation technologies can move resources between zones. Storage technologies can store resources over one or more time intervals.

a waste if it is emitted to the atmosphere, or an intermediate if it is captured stored or utilised).

As illustrated in Figure 6-3, conversion technologies take certain resources as inputs and produce others as outputs. Conversion technologies are governed by various constraints including the efficiencies, and other requirements, with which they convert the input resources to the outputs, maximum and minimum operating rates, and costs. Also included in the VWM are storage technologies, that store given resources over one or more time intervals. Storage technologies are governed by constraints including maximum and minimum storage inventory, resource requirements, etc. Finally, transmission technologies enable the transportation of resources between spatial zones: some transmission technologies (natural gas and hydrogen pipelines) also include linepack storage. In addition to these resource and technology constraints, further constraints in the VWM keep track of overall system costs, environmental impacts and other factors such as land use.

The resources and technologies in Figure 6-3 were all included in the scenario modelling for this study. The input data for these technologies was based on the data in [73]; more information is provided in the supplementary material*. Uptake of hydrogen technologies was the focus of this study, so various hydrogen technologies were modelled. Alternative energy resources and technologies were also included, such as electricity and natural gas.

Three hydrogen production value chains that were modelled in this study: reforming of methane, electrolysis (also known as power-to-gas), and gasification of biomass. Inclusion of a bioenergy production route allows for the potential for negative CO_2 emissions, if the CO_2 emitted through gasification is captured and sequestered in CO_2 storage. Design of bioenergy value chains is complex, with different pathways available including generation of electricity and heat, and the environmental impact of the value chain can depend heavily on the biomass feedstock and conversion processes used [74]. Evaluation of these issues, specific to bioenergy, is beyond the scope of this study. Here, a representative biomass to hydrogen value chain was modelled in order to explore its possible interaction with other hydrogen value chains. For more details of this value chain, see the supplementary material†.

The technologies included in the study for the utilisation of hydrogen were: combined cycle gas turbines (CCGTs) and open cycle gas turbines (OCGTs) for the conversion

*The original article supplementary material is not provided with this thesis, however information on the input data used in this chapter is given in Appendix B.

†In this thesis, see Appendix B.

of hydrogen to electricity; fuel cells and combined heat and power (CHP) plants for conversion to electricity and heat; and a range of heating technologies for the industrial, commercial and domestic sectors. Hydrogen storage technologies were also modelled: underground for interseasonal storage (salt caverns and depleted oil and gas reservoirs) and overground pressure vessels for shorter timescale storage. Hydrogen transmission pipelines with linepack storage capacity were also modelled.

Injection of hydrogen into existing gas distribution grids was also modelled, either partially or via complete conversion of the gas grid to hydrogen. Partial injection refers to the blending of hydrogen with natural gas, up to a certain limit (20% by volume in this study). This process involves minimal alterations to existing natural gas distribution grids, but requires injection equipment to ensure that the maximum allowable level of injection is not exceeded. Alternatively, "100%" hydrogen injection involves the conversion of natural gas distribution grids to hydrogen, so that they can no longer be used for natural gas. The practicalities of both of these injection options, as well as further details of how they are represented in the VWM, are provided by Quarton and Samsatli [18].

6.3.2 Scenario design

The scenarios that were modelled were designed to represent the transition of a mid-sized energy system from the present day to net-zero by 2050. The modelled system represents the Great Britain (GB) energy system. Demands for heat and electricity in the domestic, commercial and industrial sectors were modelled, that must be satisfied at all times. Any of the technologies shown in Figure 6-3 could be installed to convert primary resources into the final energy demands, although subject to their operational constraints, and incurring costs for installation and operation. Additionally, existing installed capacities of several technologies were modelled, including natural gas transmission and distribution infrastructures.

In this study GB was represented with 16 spatial zones, based on the National Grid Seven Year Statement zones [75]. Temporally, three seasons were modelled: summer, winter, and a short "peak" season (for the most extreme energy demands). Within each season, days were represented with four sub-day intervals, representing sub-day variability in resource availabilities and demands. Finally, four decadal planning intervals were modelled, allowing new investment decisions at the beginning of each decade, and long-term trends in energy demands and technology costs. The model input data used in this study, including technology data and spatio-temporal resource availabilities and demands, was based on [73]: more details can be found in the supplementary material‡.

In this study, 15 different scenarios were modelled, each with a unique configuration of decarbonisation policies and hydrogen incentives. Additionally, 23 sensitivity scenarios were modelled, exploring the effects of certain data assumptions. The policy scenarios were designed based on the information that was gathered in Section 6.2, and are separated into two groups:

1. Scenarios with policies for penalising existing technologies, in order to achieve energy system decarbonisation;
2. Scenarios with additional policies for hydrogen technologies (whilst still including policies to achieve decarbonisation).

As the scenarios that were modelled represent the GB energy system, the currency used for modelling was British pound sterling (£). In the remainder of this paper, cost data are reported in pounds. In 2019 the average exchange rate between British pounds and U.S. dollars was £1 = \$1.28 [76].

6.3.2.1 Scenarios with policies for decarbonisation

Table 6.3 gives a summary of the first set of scenarios, with policies to penalise existing technologies and achieve decarbonisation. The modelled scenarios include: one in which CO_2 was not constrained; a set of three with different CO_2 budget trajectories; and a set of three with different CO_2 tax trajectories. Apart from the "CO_2 unconstrained" scenario, the goal of the scenarios is to decarbonise by 2050 at minimum overall system cost. Although the decarbonisation target is to reach net-zero emissions, whether or not this is achieved depends on the policies that are imposed (e.g. a CO_2 tax does not guarantee the system will reach net zero by 2050, as discussed in Section 6.2.1.1).

CO_2 unconstrained scenario

In the "CO_2 unconstrained" scenario, no constraints or other policies are applied to CO_2 emissions, so the optimisation simply seeks to meet all energy demands at minimal cost, irrespective of environmental impact. This scenario gives an indication of the overall system costs and emissions in a case with no policy intervention.

‡In this thesis, see Appendix B.

Table 6.3: Details of the first set of scenarios, focussing on policies for decarbonisation. The CO_2 tax rates shown are model input values, and are therefore un-discounted.

Scenario subset	CO_2 constraint/impact	2020 - 2030	2030 - 2040	2040 - 2050	2050 - 2060
CO_2 unconstrained	None	-	-	-	-
CO_2 budgets	CO_2 budget ($MtCO_2$/yr):				
	1) "Late"	236	236	236	0
	2) "Steady"	236	160	80	0
	3) "Early"	236	100	50	0
CO_2 tax	CO_2 tax (£/tCO_2):				
	1) "Low"	54	116	177	240
	2) "Medium"	54	132	209	290
	3) "High"	54	148	241	340

CO_2 budgets scenarios

In the "CO_2 budgets" scenarios, a constraint was applied that limits the total allowable emissions in each decade:

$$\mathscr{I}^{\text{total}}_{\text{CO}_2,y} \leq B^{\text{CO}_2}_y n^{\text{yy}}_y \qquad \forall y \in \mathbb{Y} \tag{6.1}$$

In this equation, $\mathscr{I}^{\text{total}}_{\text{CO}_2,y}$, defined in Section 2 of supplementary material[§], is the total CO_2 impact (net CO_2 emissions, in $MtCO_2$) in the entire system during planning period y; $B^{\text{CO}_2}_y$ is the CO_2 budget (in $MtCO_2$/yr) in period y; and n^{yy}_y is the number of years in period y.

Three CO_2 budget scenarios were modelled with different budget trajectories, shown in Table 6.3. All cases have a budget of 236 $MtCO_2$/yr in the first decade, estimated from the fourth and fifth carbon budgets set by the Committee on Climate Change [77] for the sectors that are included in this study. The budget for the final decade was set to 0 $MtCO_2$/yr in all cases. Each case has different budgets for the intervening decades: the "steady" case represents a consistent reduction of around 80 $MtCO_2$/yr per decade, whilst the other cases represent either slower or faster decarbonisation trajectories that still reach net-zero emissions by 2050.

With minimal policy intervention, the "late" case theoretically gives the cost-optimal pathway for achieving net-zero emissions in 2050-2060. Comparison of the three cases shows the effects of different decarbonisation trajectories on the overall energy system

[§]The original article supplementary material is not provided with this thesis. For a definition of $\mathscr{I}^{\text{total}}_{\text{CO}_2,y}$, refer to the original article.

design, CO_2 emissions, and costs. These scenarios are also analogous to a CO_2 cap-and-trade scheme, assuming that the entire energy system is included in the scheme.

CO_2 tax scenarios

Three scenarios were modelled with CO_2 taxes imposed on all CO_2 emissions across the system, whilst negative emissions (e.g. from bioenergy with CCS) are rewarded at the same rate. The net cost to the system of the CO_2 tax is defined as follows:

$$\mathscr{I}^{\mathrm{CO_2tax}}_{\mathrm{Cost},y} = \mathscr{I}^{\mathrm{total}}_{\mathrm{CO_2},y} V^{CO_2}_y \frac{D^{\mathrm{OM}}_{\mathrm{Cost},y}}{D^{\mathrm{OM}}_{\mathrm{CO_2},y}} \qquad \forall y \in \mathbb{Y} \tag{6.2}$$

In this equation the total system CO_2 impact, $\mathscr{I}^{\mathrm{total}}_{\mathrm{CO_2},y}$, is multiplied by the CO_2 tax rate, $V^{CO_2}_y$, which has a pre-defined value for each decadal interval y. The final factor in Equation 6.2 relates to discounting of cost and CO_2 impacts. All annual impacts in $\mathscr{I}^{\mathrm{total}}_{iy}$ in the model include a discount factor D^{OM}_{iy}, which discounts annual impacts in period y back to the present day (for example to represent the time value of money). However, CO_2 impacts are generally not discounted (but could be in principle, for example to penalise earlier emissions, which remain in the atmosphere for longer, causing more climate damage). Therefore, the quotient $D^{\mathrm{OM}}_{\mathrm{Cost},y}/D^{\mathrm{OM}}_{\mathrm{CO_2},y}$ is included to convert the discounting of CO_2 into discounting of cost.

The net cost of the CO_2 tax, $\mathscr{I}^{\mathrm{CO_2tax}}_{\mathrm{Cost},y}$, is included in the optimisation objective function (which is a sum of all system costs), so will incentivise a reduction in CO_2 emissions. However, CO_2 emissions are not controlled directly, so achieving net-zero emissions is not guaranteed, but depends on whether the tax rate is a sufficient incentive to decarbonise.

In each scenario, the CO_2 tax rate is increased in each decade, reaching its maximum in the final decade. The tax rates that are modelled ($V^{CO_2}_y$) are given in Table 6.3 and are un-discounted values. The initial tax rate of £54/tCO_2 is taken from the National Grid FES 2019 "High" CO_2 price scenario; the rates in subsequent decades rise linearly [78].

6.3.2.2 Scenarios with policies for incentivising hydrogen

The second set of scenarios includes policies for supporting hydrogen technologies, to explore their effectiveness for encouraging hydrogen uptake. All scenarios in this set

Table 6.4: Details of the second set of scenarios, focussing on policies for incentivising hydrogen. The hydrogen FITs shown are model input values and are therefore undiscounted.

Scenario subset	H_2 constraint/incentive	2020 - 2030	2030 - 2040	2040 - 2050	2050 - 2060
H_2 injection obligations	Minimum H_2 injection (TWh/yr):				
	1) "Low"	0	25	50	100
	2) "Medium"	0	50	100	200
	3) "High"	0	75	150	300
H_2 injection FITs	H_2 injection FITs (£/MWh):				
	1) £10/MWh	0	10	10	10
	2) £30/MWh	0	30	30	30
	3) £50/MWh	0	50	50	50
H_2 boiler grants	H_2 boilers capital grant (% of capex):				
	1) 50%	0	50	50	50
	2) 100%	0	100	100	100

also include CO_2 budgets, equal to the budgets in the "steady" CO_2 budgets case in Table 6.3, to ensure that the system still reaches net-zero emissions by 2050. The policies that were modelled focus on the use of hydrogen in gas distribution grids, to be subsequently used for domestic and commercial heat.

Table 6.4 gives details of the scenarios. The policies that were modelled are based on the information in Section 6.2, and include: a set of scenarios with obligations for hydrogen injection (quantity-driven incentives); a set of scenarios with feed-in tariffs for hydrogen injection (price-driven incentives); and a set of scenarios with capital grants for hydrogen boilers.

Hydrogen injection obligations

The first set of hydrogen-focussed scenarios use a quantity-driven incentive. A constraint is imposed stating that the total amount of hydrogen injected into gas grids in a given decade y must exceed the minimum required level:

$$H_y^{\text{inj}} \geq H_y^{\text{min}} \qquad \forall y \in \mathbb{Y} \tag{6.3}$$

Where H_y^{min} is the minimum required level of hydrogen injection (the hydrogen injection obligation, in TWh/yr), and H_y^{inj} is the total amount of hydrogen injected into gas grids per year in period y, given by:

$$H_y^{\text{inj}} = 10^{-6} \sum_{zhdt, p \in \mathbb{P}^{\text{inj}}} \left(n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \mathscr{P}_{pzhdty} \alpha_{\text{H}_2,py} \right) \qquad \forall y \in \mathbb{Y} \tag{6.4}$$

In this equation, hydrogen injection may be via partial injection, or completely converted gas grids: these technologies make up the subset $p \in \mathbb{P}^{\text{inj}}$. $\mathscr{P}_{pzhdty}$ is the total operating rate of all technologies of type p in spatial zone z during a given time interval (hour h of day type d in season t of decade y). $\alpha_{\text{H}_2,py}$ is the rate at which a single technology p consumes or produces hydrogen: therefore the product of $\mathscr{P}_{pzhdty}$ and $\alpha_{\text{H}_2,py}$ (for $p \in \mathbb{P}^{\text{inj}}$) is the total rate of injection of hydrogen in a given time interval (in MW). Finally, the parameter n_h^{hd} gives the duration of each hourly interval h, n_d^{dw} gives the number of day types d in a week, and n_t^{wt} gives the number of weeks in season t.

The optimisation seeks the system with the lowest overall cost that meets this constraint. In practice, these scenarios could represent a tradeable obligation certificate scheme, where each gas supplier has an obligation to inject a level of hydrogen into the gas grid. Three scenarios are included in this set, with required injection levels in the final decade of 100 TWh/yr, 200 TWh/yr and 300 TWh/yr respectively. There is no minimum level in the first decade, and the minimum level rises progressively in the following decades. For comparison, the energy supplied to the GB natural gas distribution grid in 2019 was approximately 480 TWh [79].

Hydrogen injection feed-in tariffs

The second set of scenarios use a price-driven incentive: a feed-in tariff (FIT) is paid for each MWh of hydrogen injected into the gas distribution grid. The FIT is paid for either partial injection or 100% injection into converted natural gas distribution grids. The FIT payment acts as a revenue to the system, therefore has a negative value when included in the optimisation objective function, which is the minimisation of total cost. The total cost impact of FIT payments can thus be defined as follows:

$$\mathscr{I}_{\text{Cost},y}^{\text{FIT}} = -H_y^{\text{inj}}\, V_y^{\text{FIT}}\, D_{Cost,y}^{\text{OM}} \qquad \forall y \in \mathbb{Y} \tag{6.5}$$

In this equation, H_y^{inj} is the total hydrogen injected per year in period y, as defined in Equation 6.4, V_y^{FIT} is the value of a FIT payment (in £/MWh), and $D_{Cost,y}^{\text{OM}}$ is the discount factor that discounts the annual costs/payments in period y back to the present day. In the model, the FIT payments are seen as a system revenue and are included in the optimisation objective function. In reality, this FIT payment would be an additional revenue to the gas supplier, and would be paid by the government (or eventually added to consumer gas bills).

Three scenarios were modelled with different FITs. In each scenario, no FIT is paid in the first decade, followed by a constant FIT in the three remaining decades. The modelled FITs were chosen based on previous work, where FITs of up to £50/MWh were found to be sufficient to incentivise partial hydrogen injection into gas grids [18]. In this study, the FIT has been extended to also apply to 100% hydrogen injection.

Hydrogen boiler capital grants

Finally, scenarios were modelled with direct capital grants for domestic and commercial hydrogen boilers. Within the VWM, this policy was modelled as a reduction in the capital cost of the boiler technologies (which would thus reduce the overall cost in the optimisation objective function). In practice, this cost would be covered by the government. In both cases, the grants are available in the third and fourth decades. The grant is worth 50% of the boiler capex in the first case, and 100% of the boiler capex in the second case.

6.3.2.3 Sensitivity scenarios

In addition to the scenarios presented above, a series of sensitivity scenarios were modelled, exploring the effects of two key assumptions. Full details of these scenarios are provided in the supplementary material¶.

Discount rate

Given that the optimisation process includes decisions and costs over several decades, the net present cost approach is used, where future costs are discounted to the present day. This discounting reflects the time value of money and means that future impacts have a lower weighting in the overall objective function than present-day impacts.

¶The original article supplementary material is not provided in with this thesis, however details of the sensitivity scenarios modelled for this study are given in Appendix D.

The discount rate may affect scenario results. For example, Emmerling et al. [80] assessed the impacts of discount rates ranging between 1% and 8% on decarbonisation outcomes in integrated assessment models and found that lower discount rates resulted in more action sooner and less need for NETs in the future. For related reasons, Stern [81] proposed that a discount rate of 0.1% be used when modelling the economics of climate change.

A discount rate of 3.5% was used for cost impacts in the main scenarios in this study, in line with UK government guidance [82]. However, sensitivity scenarios were also modelled with discount rates of 0.1% and 8%. As the discount rate is most likely to affect decarbonisation decisions, such as when to invest in decarbonisation and the impacts of CO_2 prices, the discount rate sensitivities were performed for the "decarbonisation" scenarios detailed in Table 6.3.

Electric heat pump coefficient of performance

Electric heat pumps are seen as a valuable option for heat decarbonisation due to their high coefficient of performance (COP); Quarton and Samsatli [18], for example, found that electric heat pumps may be preferred to conversion of gas grids to hydrogen due to the greater energy efficiency from production end-use. However, there is some uncertainty in the COP that may be achievable by electric heat pumps. In the main scenarios in this study, COPs of 2.5 and 4 were assumed for domestic heat pumps and commercial heat pumps, respectively. Sensitivity scenarios were modelled with a COP of 2 for both domestic and commercial heat pumps, to determine whether this lower COP would affect electric heat pump uptakes and, consequently, hydrogen uptake. These sensitivities were performed for the scenarios with hydrogen-focussed policies detailed in Table 6.4.

6.3.3 Implementation

The VWM was implemented in AIMMS (Advanced Interactive Multidimensional Modeling System) and solved with the CPLEX solver. Each scenario includes approximately 200,000 variables, of which around 4,000 are integer variables, and 330,000 constraints. The optimisation was performed on a workstation with 10 cores and 128 GB RAM. Each scenario took around 30 hours to solve with an optimality tolerance of 2%.

6.3.4 Interpretation of cost results

All scenarios in this study consider the transition of the GB energy system over four decades from 2020 with the optimisation objective of minimising system net present cost. The system cost includes all of the costs incurred in the utilisation of the resources and installation and operation of the technologies shown in Figure 6-3, thus representing the overall cost to society, including both costs incurred by energy producers (e.g. installation and operation of a power plant), and costs incurred by consumers (e.g. installation and operation of a boiler in the home or business). Although system cost is useful for comparing the overall cost of different scenarios, additional metrics are described in this section that can be used to explore costs in more detail, including the costs for particular policies or individuals.

Some of the implications of discount rates for optimisation modelling were described in Section 6.3.2.3. Discounting of future costs also has implications when comparing model results and policies from different decades. In this study, unless otherwise stated, the cost results that are reported are the present-day, discounted costs. However, undiscounted values are reported in some cases where they are more relevant.

6.3.4.1 Average CO_2 cost

The average CO_2 cost metric was used to compare costs and CO_2 emissions between scenarios. For a given scenario, the overall system costs and emissions are compared to a reference case (the unconstrained CO_2 case), to give the additional cost for each tonne of CO_2 that is saved:

$$C^{\mathrm{CO2,avg}} = \frac{\sum_y \mathscr{I}^{\mathrm{total}}_{\mathrm{Cost},y} - I^{\mathrm{REF}}_{\mathrm{Cost}}}{I^{\mathrm{REF}}_{\mathrm{CO_2}} - \sum_y \mathscr{I}^{\mathrm{total}}_{\mathrm{CO_2},y}} \tag{6.6}$$

In this equation $\mathscr{I}^{\mathrm{total}}_{\mathrm{Cost},y}$ and $\mathscr{I}^{\mathrm{total}}_{\mathrm{CO_2},y}$ are the total cost and CO_2 impacts in each decade y for the scenario in question, discounted to present day values; in Equation 6.6 they are summed over all decades y to give total values for the entire time horizon. $I^{\mathrm{REF}}_{\mathrm{Cost}}$ and $I^{\mathrm{REF}}_{\mathrm{CO_2}}$ are the equivalent total cost and CO_2 impacts over the entire time horizon for the reference case (the unconstrained CO_2 case). As a result, a value for the average cost of CO_2 savings is obtained, which has units of £/tCO_2 and is discounted to the present day.

6.3.4.2 Hydrogen policy cost-effectiveness

A similar metric to the average CO_2 cost was used to assess the cost-effectiveness of policies for incentivising hydrogen. This metric compares overall system costs and hydrogen uptake between a given scenario and a reference scenario. Hydrogen uptake is measured in terms of total hydrogen production and is calculated as follows:

$$H_y^{\text{prod}} = \sum_{zhdt,p\in\mathbb{P}^{\text{H}}} \left(n_h^{\text{hd}} n_d^{\text{dw}} n_t^{\text{wt}} \mathscr{P}_{pzhdty} \alpha_{\text{H}_2,py} \right) \qquad \forall y \in \mathbb{Y} \tag{6.7}$$

This equation has a similar definition to Equation 6.4 but is summed over *all* hydrogen-producing technologies, denoted by the subset $p \in \mathbb{P}^{\text{H}}$. Hence, total hydrogen production in decade y is calculated by summing the hydrogen produced by each technology p in spatial zone z, during time interval hdt.

In this case, the reference scenario is the "steady" CO_2 budgets scenario, which reaches net-zero emissions by 2050 and has no specific hydrogen incentives. The hydrogen policy cost-effectiveness is defined as the increase in overall system cost compared to the reference case, for each additional MWh of hydrogen produced over the course of the time horizon. It is given by the following equation:

$$C^{\text{H}_2,\text{avg}} = \frac{\sum_y \mathscr{I}_{\text{Cost},y}^{\text{total}} - I_{\text{Cost}}^{\text{REF}}}{\sum_y H_y^{\text{prod}} - H^{\text{REF}}} \tag{6.8}$$

where H^{REF} is the total hydrogen produced over the time horizon in the reference case. $C^{\text{H}_2,\text{avg}}$ signifies the effect on the discounted overall system cost of the increased hydrogen usage in the system (units of £/MWh).

6.3.4.3 Marginal CO_2 cost

A marginal CO_2 cost metric was used to represent the change in overall system cost for a change in total system emissions of 1 tCO_2, calculated using the shadow price property within AIMMS. The shadow price of a constraint within AIMMS is defined as "the marginal change in the objective value with respect to a change in the right-hand side (i.e. the constant part) of the constraint" and is calculated by the optimisation solver [83].

Therefore for this study, the shadow price of the CO_2 budget constraint (shown in

Equation 6.1) in a given decade y gives the change in the overall system cost (the objective function) that arises if the allowable level of emissions in a decade is increased by 1 tCO_2. This value is described as the marginal cost of CO_2, $C_y^{CO_2,\mathrm{marg}}$. As a different CO_2 budget can be imposed in each decade, $C_y^{CO_2,\mathrm{marg}}$ has a different value for each decade.

Scenarios with enforced CO_2 budgets may represent a CO_2 cap-and-trade scheme, assuming that: all CO_2 emissions across the entire system (e.g. including domestic emissions) are included in the scheme; there is perfect operation of the scheme; and emissions allowances can be efficiently traded between emitters. The marginal CO_2 cost, $C_y^{CO_2,\mathrm{marg}}$, represents the cost of an emitter reducing their emissions by 1 tCO_2, discounted to present day values. The price at which an emitter would be willing to purchase a CO_2 allowance is likely to be equal to this value, although un-discounted in order to represent the actual price paid at that time. Therefore the estimated CO_2 allowance trading price is given by:

$$T_y^{CO_2} = \frac{-C_y^{CO_2,\mathrm{marg}}}{D_{\mathrm{Cost},y}^{\mathrm{OM}}} \qquad \forall y \in \mathbb{Y} \tag{6.9}$$

6.3.4.4 Policy cost

Some scenarios in this study include fiscal intervention by the government: in particular, CO_2 taxes represent a cost to the energy system (and a revenue to the government), whilst hydrogen FITs are a revenue for the energy system (but a cost to the government). The total financial values of these interventions, in (discounted) present day terms, have already been defined in Equation 6.2 (CO_2 tax) and Equation 6.5 (hydrogen FITs), and give an indication of the scale of government intervention in a scenario.

Although the financial values of these interventions are included in the optimisation objective function, they are removed from the overall system costs that are presented in the results in this study. This means that scenarios can be compared without financial interventions affecting the overall system cost: any differences in costs are caused by differing decarbonisation pathways and investment decisions that arise from the policies, rather than the policies themselves. This effectively assumes that the policy is revenue-neutral, in that any costs or revenues imposed on the energy system by the government would be balanced by other policies elsewhere.

6.3.4.5 Consumer costs

To assess the consumer impact of different decarbonisation pathways, two 2050 consumer heating bills were estimated from the value chain optimisation results: one assuming electrification and the other hydrogen. Although the optimisation minimises net present (i.e. discounted) costs, the typical consumer's energy bill was post-calculated using un-discounted costs, as this what the consumer would actually pay.

The value chain optimisation results include the numbers of technologies installed in each decade, their operating regimes, and the total costs of installing and operating the technologies. Therefore the average unit cost (£/MWh) for producing a given resource, such as hydrogen, electricity or heat, can be calculated, although assumptions are required when technologies and infrastructures are shared between multiple value chains.

The electrification of heating scenario was calculated from the "steady" CO_2 budgets case, in which the majority of heating is electrified by 2050, and represents an approximate annual heating bill for a typical domestic consumer using an electric heat pump. The unit cost of electricity production was calculated from the sum of all of the electricity production technologies in the scenario results, including wind power, solar PV, nuclear power and natural gas power plants. The unit costs for electricity transmission and distribution were each based on the associated technologies within the VWM, and assumed to be divided equally between each MWh of electricity flowing through the networks. Annual electricity consumption was taken from the average consumption of a domestic electric heat pump in the final decade of the scenario.

Other fixed costs that would usually be included in a consumer energy bill, such as supplier overheads, are not included in the VWM, so were assumed to be the same, per MWh of electricity, as in present-day electricity bills. These data were taken from Ofgem [84]. Finally, the annualised cost to the consumer of installing the heat pump and any other necessary in-home upgrades was calculated, assuming that the initial capital investment would be annualised over the lifetime of the heat pump. Although these costs would not typically be included in an energy bill, they still represent a consumer cost, therefore it is important consider them when comparing heating scenarios.

The hydrogen heating scenario was calculated from the "high" hydrogen injection obligations case, where there is a required minimum injection of hydrogen into the gas grids of 300 TWh/yr in 2050-2060. The annual heating bill was calculated in a similar manner to the electrification bill: unit costs were calculated for hydrogen production, transmission, storage and distribution. The hydrogen production cost was calculated from the costs of the hydrogen production technologies in the scenario results, including the cost of CCS, which was assumed to be shared between all users, including SMR plants and other natural gas users. The costs of hydrogen transmission and storage infrastructure from the scenario results were assumed to be shared between domestic, commercial and industrial consumers of hydrogen. Likewise, hydrogen distribution costs, including conversion of existing gas grids to hydrogen, were assumed to be shared between all users of distributed hydrogen, based on their energy consumption. Other fixed costs were assumed to be the same as in present-day natural gas bills [85]. Finally, annualised costs of a new hydrogen boiler and any necessary in-home safety checks for conversion from natural gas to hydrogen were included.

For comparison, a benchmark present-day bill for a consumer using natural gas for heating was also estimated from Ofgem [85] and BEIS [86] data. For equivalence with the other scenarios, annualised costs for a new natural gas boiler were also included.

6.4 Results and discussion

Results from the optimisation scenarios are presented and discussed in this section. The results from the scenarios with policies for penalising existing technologies, to achieve system decarbonisation, are discussed first. Then, the uptake of hydrogen in the scenarios is considered, including scenarios with and without additional policies to support hydrogen technologies. Finally, the scenario results are used to consider the impact on consumer costs of different decarbonisation pathways, in particular electrification vs. conversion of gas grids to hydrogen.

6.4.1 Policies for decarbonisation

Figure 6-4 shows the cumulative costs and CO_2 emissions for a selection of scenarios. The "CO_2 unconstrained" scenario has the lowest overall cost but the highest emissions, with annual emissions increasing by the final decade, due to rising energy demands and a continued high contribution of natural gas to the energy supply. The scenarios with CO_2 budgets and CO_2 taxes all have lower CO_2 emissions, but with different decarbonisation trajectories and costs.

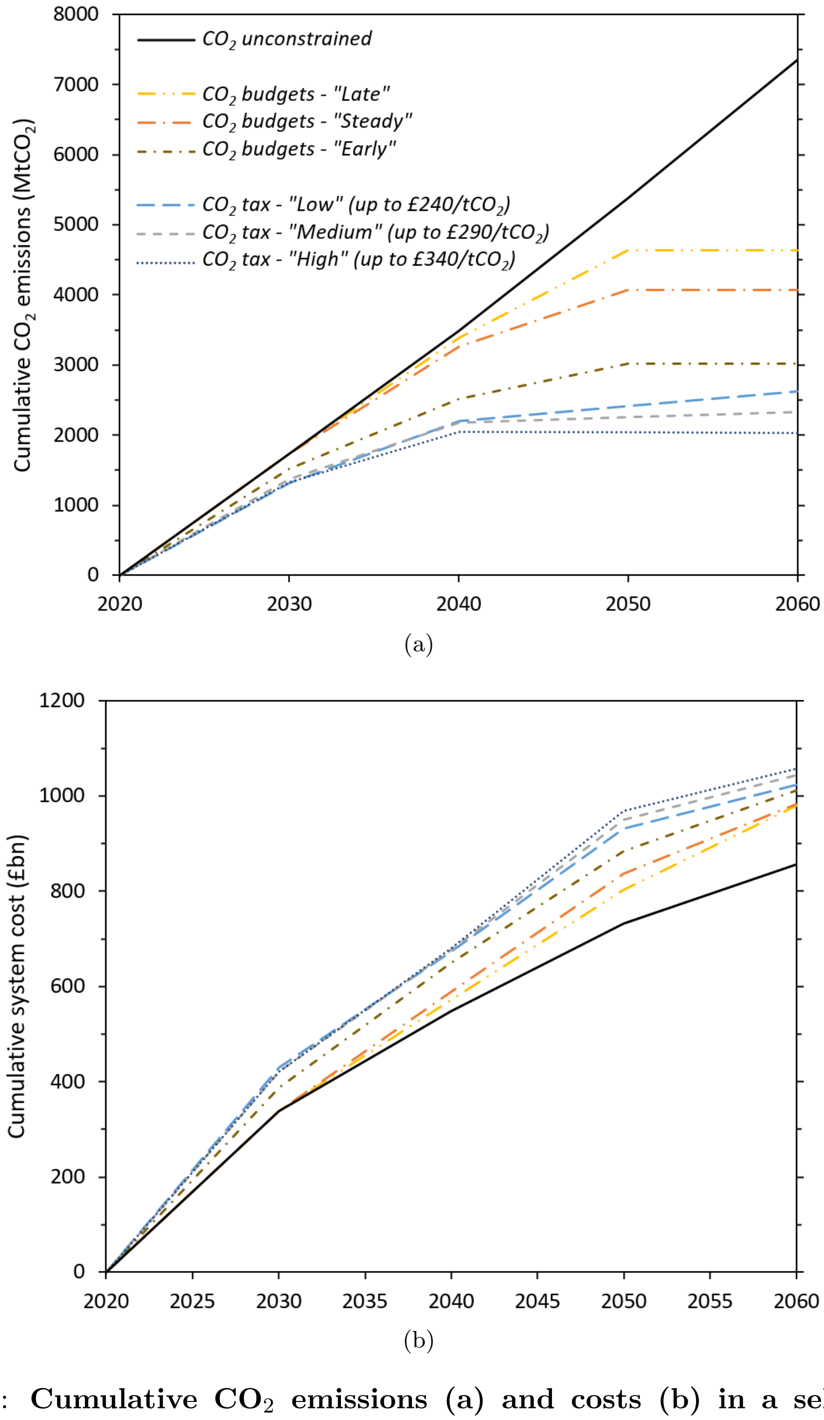

Figure 6-4: **Cumulative CO_2 emissions (a) and costs (b) in a selection of scenarios.** Costs are overall system costs, discounted to 2020.

6.4.1.1 CO_2 budgets

The emissions limits in the CO_2 budgets scenarios are strictly controlled, so all achieve net-zero emissions in the final decade (indicated by zero slope in the final decade of Figure 6-4(a)). However, the different budget trajectories in each case result in different overall levels of emissions and net-present (discounted) system costs. As Figure 6-4(a) shows, cases with more stringent budgets in the early decades result in significantly lower emissions overall. For example, the total CO_2 emitted over four decades in the "early" decarbonisation case is more than 1.6 $GtCO_2$ lower than in the "late" decarbonisation case.

Despite the differences in total CO_2 emitted, the range in costs of the different CO_2 budget scenarios is small: for example, the "early" decarbonisation case is only 3% more expensive than the "late" decarbonisation case. As Figure 6-4(b) shows, the cases with more stringent CO_2 budgets in the earlier decades incur greater costs in these decades, but by the final decade costs converge. This suggests that the overall costs of decarbonisation arise predominantly from shifting the system to net-zero, and the timescales over which this transition is achieved is not as significant.

As a result, if the objective is to minimise the total CO_2 emitted into the atmosphere, earlier decarbonisation is more cost-effective (per unit of prevented CO_2 emissions). Comparing the CO_2 budgets scenarios to the CO_2 unconstrained scenario, the "late" decarbonisation case saves a total of 2.7 $GtCO_2$, whilst the "steady" and "early" cases save 3.3 $GtCO_2$ and 4.3 $GtCO_2$ respectively. Since each case has similar overall costs, this means that the "late" case has a higher average cost of CO_2 saved: £45/tCO_2 compared to the unconstrained case, whilst the "steady" and "early" cases have average CO_2 costs of £38/tCO_2 and £36/tCO_2 respectively.

If the CO_2 budgets were to represent a CO_2 cap and trade scheme, the approximate CO_2 allowance trading price can be calculated from Equation 6.9. For net-zero emissions in 2050-2060, the trading price would be approximately £1720/tCO_2 in the "late" decarbonisation case, £600/tCO_2 in the "steady" case, and £460/tCO_2 in the "early" case. Although these potential CO_2 trading prices are very high, it is important to note that they reflect the cost of removing the final tonne of CO_2 of emissions from the system, and the majority of emissions can be removed at lower cost.

The wide range in CO_2 allowance trading prices between the cases is also significant. The very high trading price, in excess of £1700/tCO_2, occurs in the "late" case, which has no decarbonisation action until the final decade; the final trading prices are much lower in the cases that have more stringent CO_2 budgets in the preceding decades. This shows that with more decarbonisation early on, a more gradual transition to net-zero can be achieved, and the costs are shared over multiple decades. As a result, the final costs of achieving net-zero are lower, and the resulting CO_2 trading price is more stable.

6.4.1.2 Carbon tax

Results from the CO_2 tax scenarios can also be seen in Figure 6-4. Only the "high" taxation case achieves net-zero by 2050-2060, suggesting that a CO_2 tax rate greater than £300/tCO_2 is necessary to incentivise the system to achieve net-zero emissions in 2050.

As Figure 6-4(a) shows, the CO_2 tax scenarios typically deliver greater levels of decarbonisation in the early decades than the CO_2 budget scenarios (since the cumulative emissions are lower). Clearly this result depends on the modelled CO_2 tax trajectory, with higher taxes leading to greater emissions reductions. The CO_2 tax trajectories that were modelled in this study were linear between the first and last decades. This result shows that lower CO_2 taxes can incentivise initial emissions reductions, when the cost of doing so is lower, but an increasing tax rate is necessary as the net-zero target is approached. This emphasises that stronger policy intervention earlier can be more effective for reducing the total amount of CO_2 emitted.

As was discussed in Section 6.4.1.1, greater levels of decarbonisation early on result in a lower final marginal cost for achieving net-zero emissions. This explains why the required CO_2 tax rate for achieving net-zero (more than £300/tCO_2) is lower than the CO_2 trading prices estimated from the CO_2 budgets scenarios (£460/tCO_2 or more). With lower CO_2 tax rates in the early decades, a higher final CO_2 tax is likely to be required to achieve net-zero.

Figure 6-4(b) shows that the CO_2 tax scenarios are more expensive than the CO_2 budget scenarios. These results do not include the cost of the CO_2 tax itself: it is assumed that the government would re-invest this tax revenue into the energy system. Therefore for reaching a net-zero energy system by 2050, CO_2 taxes appear to be more expensive overall, with an extra cost of £78bn in the "high" CO_2 tax case compared to the "late" CO_2 budget case. Nonetheless, given the lower cumulative level of emissions in the CO_2 tax cases, the average costs per tonne of CO_2 averted are similar for the CO_2 tax cases and the CO_2 budget cases, with a range of £35–38/tCO_2 for the CO_2 tax cases, compared to £36–45/tCO_2 for the CO_2 budget cases. The total system cost (or government revenue) of the CO_2 tax over all decades (Equation 6.2) ranges from £125bn in the "high" tax case to £156bn in the "low" tax case.

6.4.1.3 Effect of discount rate

All the scenarios described so far were modelled with a discount rate of 3.5%. However, a sensitivity study was also performed in which the same scenarios were modelled with discount rates of 0.1% and 8%. Detailed results from these scenarios are provided in the supplementary material‖ and are summarised here. The discount rate determines the importance of future costs relative to present day costs. With a discount rate of 0.1%, future costs have almost equal weighting to present-day costs in the optimisation objective function, whilst with higher discount rates the importance of future costs falls.

In the case of CO_2 budgets, this means that with higher discount rates, investment in decarbonisation is delayed until it is essential, as the associated costs are seen to reduce. The level of voluntary early decarbonisation, i.e. the reduction in CO_2 emissions in a given decade beyond what is required by the CO_2 budget, is notably higher in the cases with a discount rate of 0.1% than the cases with higher discount rates. Examples of this voluntary early decarbonisation include earlier investment in renewable electricity generation and long-life infrastructure such as electricity distribution networks. As a result, the cases with a discount rate of 0.1% have lower total CO_2 emissions than the cases with a discount rate of 3.5%: 21% lower in the "late" CO_2 budget case and 11% lower in the "steady" case.

The discount rate also reduces the importance of the costs arising from future CO_2 taxes in the optimisation objective function, thus reducing the impact of future CO_2 taxes. This can be seen in the sensitivity study results: with a discount rate of 3.5%, a CO_2 tax of £340/tCO_2 was required in 2050-2060 to achieve net-zero emissions, but this was achieved with a CO_2 tax of £290/tCO_2 when a discount rate of 0.1% was used.

Finally, given that most decarbonisation spending occurs in later decades, the effect of the discount rate in all scenarios is to reduce the apparent costs of this decarbonisation. This can be seen in the average costs of CO_2 reductions compared to the respective reference cases (with no decarbonisation policies). From all of the CO_2 tax and CO_2 budget cases, the average cost of CO_2 is £80–103/tCO_2 for a discount rate of 0.1%; £35–45/tCO_2 for a discount rate of 3.5%; and £9–12/tCO_2 for a discount rate of 8%.

These results show the importance of the discount rate when considering investment decisions over long time periods. Whilst it is difficult to know what the most appropriate discount rate is for a given assessment, it is essential that the discount rate is taken into consideration when interpreting scenario results.

‖In this thesis, see Appendix D.

6.4.2 Policies for incentivising hydrogen

The scenarios for supporting hydrogen technologies are studied in more detail in this section, including the resulting energy system design and the role of hydrogen. First, the uptake of hydrogen in a scenario without any specific hydrogen policies is considered. This is then compared to further scenarios with different policies supporting hydrogen technologies.

6.4.2.1 Net-zero system without hydrogen incentives

To compare the effectiveness of policies supporting hydrogen technologies, first a scenario is considered in which no specific hydrogen policies were included. The "steady" CO_2 budgets scenario is used for this purpose, as this represents the most probable decarbonisation pathway, reaching net-zero emissions by 2050 with equal reductions in each decade. In any case, the details of the final energy system in the other CO_2-budgets scenarios are similar. Figure 6-5 shows a Sankey diagram of the annual energy flows in the final decade of the "steady" CO_2 budgets scenario.

The optimised net-zero energy system includes a balanced mix of electricity supply. Offshore wind and nuclear power are the main contributors, supplying 43% and 25% of annual supply respectively. Natural gas with CO_2 capture makes up 22% of annual supply (all captured CO_2 is sequestered offshore). A small amount of electricity balancing is provided at peak times by natural gas without CO_2 capture and hydrogen combined heat and power (CHP): each contributes around 1% to annual electricity supply. The heat from the hydrogen CHP is used for commercial heating applications.

The optimal decarbonised heat supply is less diverse, with 87% of domestic and commercial heat demands being satisfied by electric heat pumps. As found in previous work, electric heat pumps appear in the optimal heat supply chain because the heat pump COP results in a high heat supply chain efficiency compared to the alternatives [18]. Given the prevalence of electric heat pumps in the scenario results, a sensitivity study was performed in which lower heat pump COPs were assumed. This had some impact on electric heat pump uptake but they were still the preferred technology, satisfying 73% of domestic and commercial heat demands in 2050-2060; more details are provided in the supplementary material**. Other than electric heat pumps, the other main contribution to commercial heating is from natural gas CHP with CO_2 capture. Industrial heating is shared between electricity (54%) and hydrogen (44%).

**In this thesis, see Appendix D.

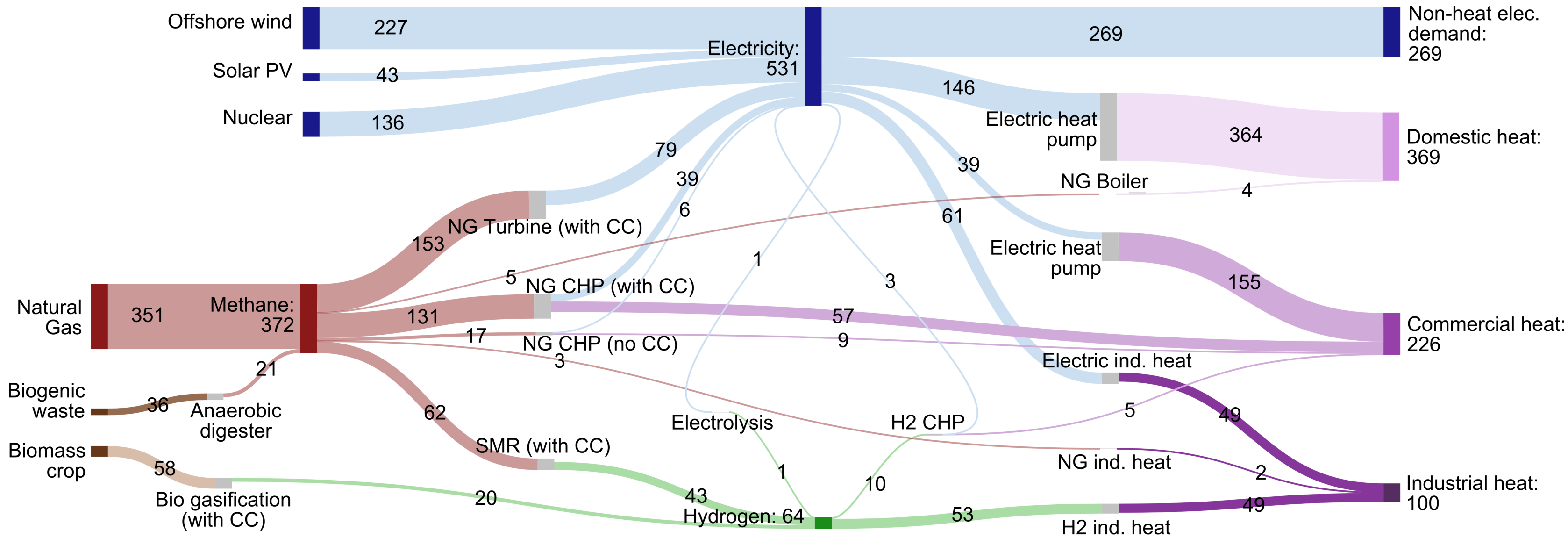

Figure 6-5: **Sankey diagram of annual energy flows in a net-zero energy system in 2050-2060.** The results shown are from the "steady" CO_2 budgets scenario. The numbers denote energy flows in TWh/yr, and flows smaller than 1 TWh/yr are not shown.

The role of hydrogen in the optimised net-zero system is fairly limited, with an annual supply of only 64 TWh/yr. The main role for hydrogen is for industrial heat, although some is used in CHP, mostly at peak times. Hydrogen supply is predominantly from SMR with CO_2 capture (67%). Bioenergy also makes up 31% of the hydrogen supply, which utilises almost all of the primary biomass available. The bioenergy-to-hydrogen value chain is responsible for 2% of final energy demands and delivers a total of 12 $MtCO_2$/yr of negative emissions. Electrolysers are used to convert excess renewable electricity to hydrogen. However, with large electricity demands for heating, there is limited low-cost electricity available. Therefore, hydrogen production from power-to-gas contributes only 1% of the annual total. Although this contribution of hydrogen is relatively small, it arises without any specific policy support.

6.4.2.2 Effect of hydrogen incentives

Various scenarios with incentives for hydrogen have been modelled, including: obligations for a minimum level of hydrogen injection into the gas grid, FITs for each MWh of hydrogen injected into the gas grid, and capital grants for hydrogen boilers. Each of these scenarios also included CO_2 budgets, matching the budgets in the "steady" CO_2 budgets case, to ensure that the system reaches net-zero emissions by 2050.

Figure 6-6 shows details of total hydrogen production and consumption in each decade of each scenario. The "steady" CO_2 budgets case is also included, representing the comparative scenario in which no hydrogen incentives are included.

As was described in Section 6.4.2.1, there is some hydrogen usage in the "steady" CO_2-budgets case, without any specific hydrogen incentives. This is focussed on the industrial sector and only arises in the final decade, when the net-zero CO_2 budget is in place.

The hydrogen injection obligations scenarios, where a minimum level of injection is enforced, have a greater uptake of hydrogen. In these scenarios, most hydrogen is produced from SMR with CCS and is used for domestic and commercial heating, supplied through natural gas distribution grids that have been converted to hydrogen. Total hydrogen usage rises with the gas grid injection obligation in each decade. Further details of the "high" hydrogen injection obligations case are shown in Figure 6-7 to give an indication of the hydrogen value chains used.

Figure 6-7 shows that hydrogen technologies are installed in most zones in 2050-2060, with most hydrogen production (via SMR with CCS) focussed in Central and Northern

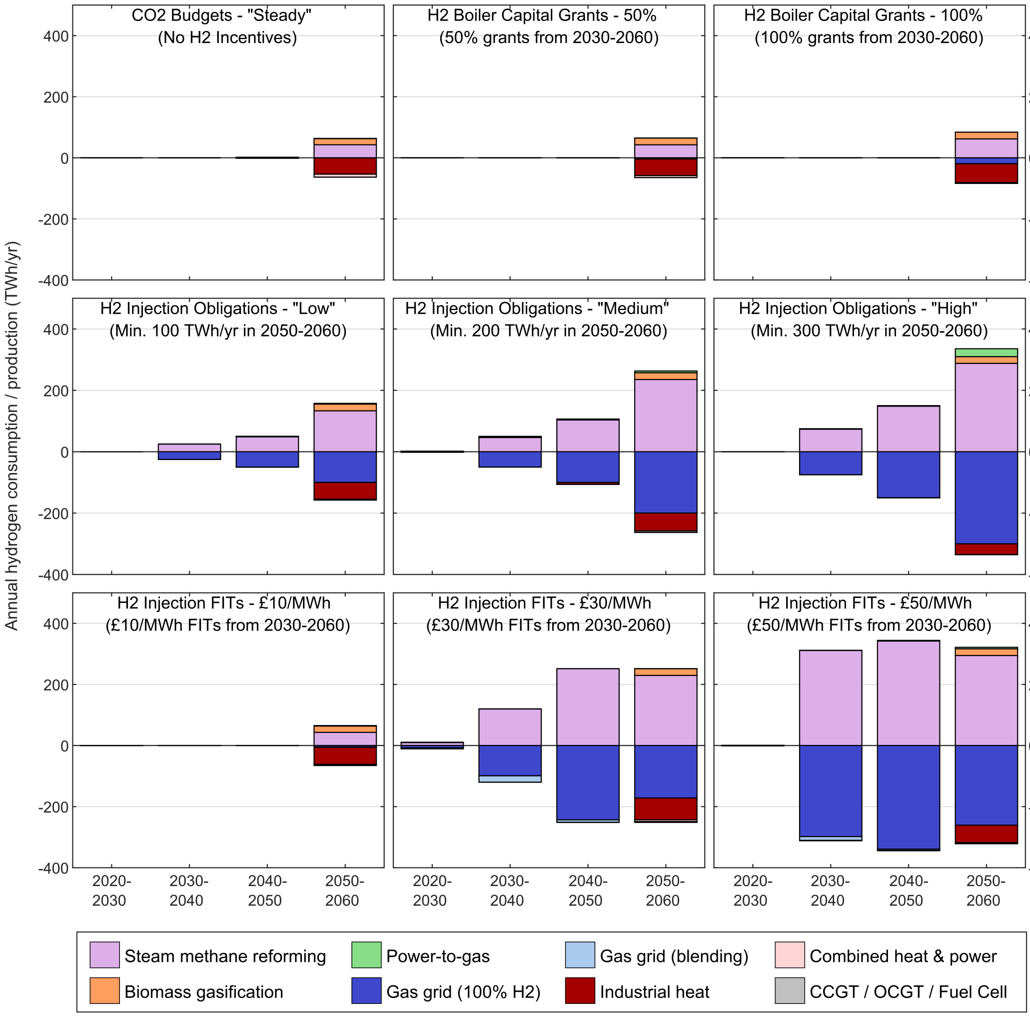

Figure 6-6: **Hydrogen production and consumption by technology or application in each decade, for each scenario.** Positive values denote hydrogen production, negative denote consumption.

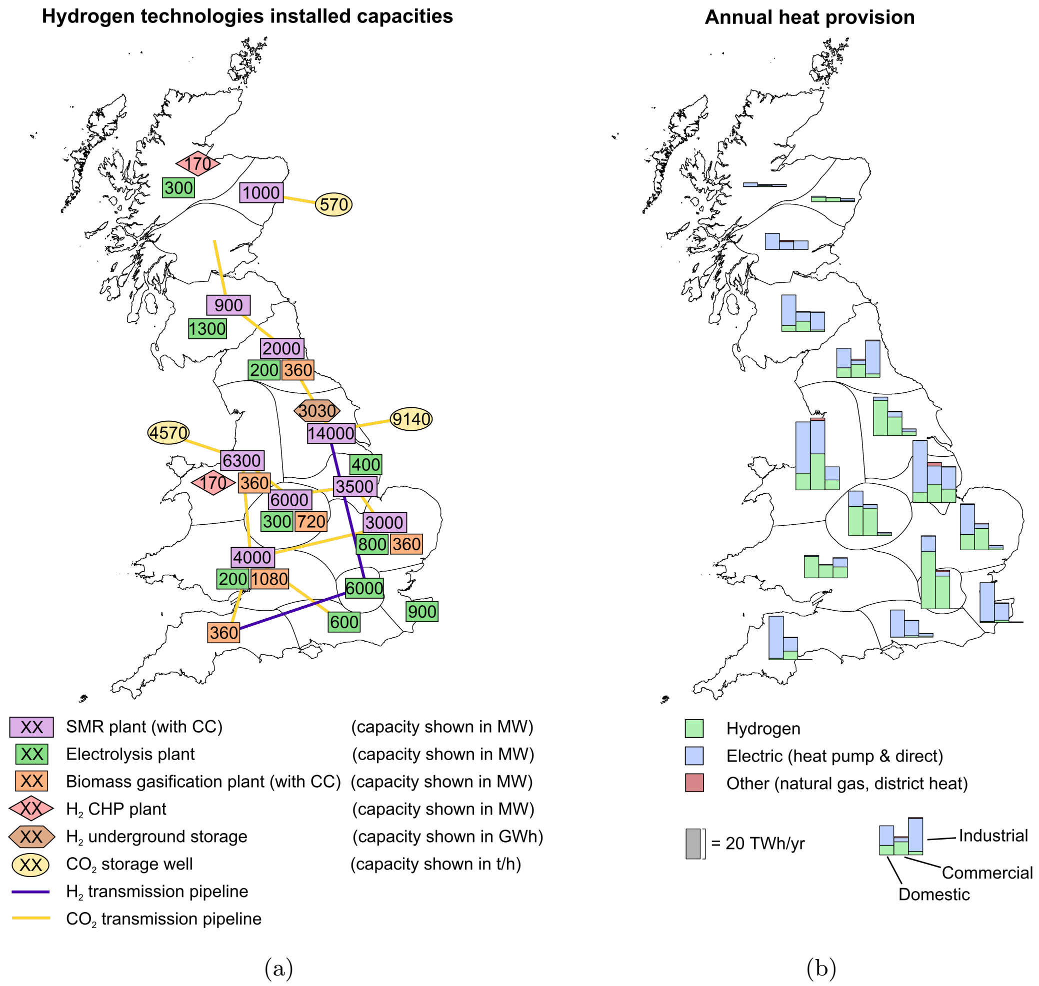

Figure 6-7: **Details of the energy system in the scenario with a minimum of 300 TWh/yr of hydrogen injection in 2050-2060 ("high" hydrogen injection obligations case).** (a) Map of installed capacities of hydrogen and related technologies in each spatial zone in 2050-2060; some technologies are not shown, including the natural gas transmission system, electricity generating technologies and hydrogen pressure vessel storage. (b) Map of annual heat provision in each spatial zone in 2050-2060; the columns in each zone represent domestic, commercial and industrial heating respectively from left to right.

England. Consequently, there is greater use of hydrogen for heating in these zones, via converted natural gas distribution grids. Further from the centre of the country, hydrogen uptake is lower, and electrification of heating is preferred. However, many zones still have power-to-gas installations, with a total installed capacity of 11 GW. The power-to-gas absorbs excess electricity at off-peak times and either feeds hydrogen into the gas grid or uses it in industrial or CHP plants.

A total storage capacity of over 3 TWh of underground hydrogen storage is installed in the system, which helps to compensate for the large seasonal variations in demand for hydrogen for heating. Although hydrogen pressure vessel storage is not shown in Figure 6-7, it is installed in almost all zones, with a total storage capacity of 260 GWh. This is used to balance within-day imbalances in hydrogen supply and demand. There is an increased need for within-day storage for hydrogen compared to an equivalent natural gas system, because a natural gas system can utilise the linepack flexibility of its transmission and distribution pipelines to a greater extent. Due to the lower energy density of hydrogen, the linepack flexibility (storage capacity) of a pipeline may be 70-83% lower with hydrogen than with natural gas under the same operating conditions [18].

As Figure 6-6 shows, hydrogen injection FITs are also effective for incentivising increased hydrogen usage. A FIT of £10/MWh is insufficient to incentivise any further hydrogen usage but FITs of £30/MWh and £50/MWh result in a significant increase. In these cases, FITs are available from 2030 onwards, causing a greater uptake of hydrogen from this date onwards. In the final decade of the £50/MWh case, 261 TWh/yr of hydrogen is used in converted gas grids, 57 TWh/yr is used in industry, and 4 TWh/yr is used in either hydrogen turbines or CHP plants.

Partial injection of hydrogen into gas grids is also rewarded by the FIT, and has greatest uptake in the early decades. For example in the £50/MWh case, 12 TWh/yr of hydrogen is blended into the natural gas distribution network in 2030-2040, representing an average injection of 19 vol.% over the entire year. However, due to the more stringent CO_2 budgets in later decades, natural gas usage is reduced, so there is little opportunity for partial hydrogen injection. Capital grants for hydrogen boilers are less effective for incentivising hydrogen. With 100% capital grants in place, 19 TWh/yr of hydrogen is used in gas grids, 62 TWh/yr is used in industry, and 2 TWh/yr is used in CHP plants. Capital grants of 50% have a negligible impact on hydrogen usage.

There is little variation between scenarios regarding how hydrogen is produced or used. All scenarios have a similar level of hydrogen usage in industry in the final decade, of around 60 TWh/yr (which also exists when no hydrogen-specific incentives are included). Otherwise, hydrogen usage is focussed on the gas grid (unsurprising, given that this is the focus of the policy incentives). Although SMR with CCS is preferred for most hydrogen production, biomass gasification consistently provides around 21 TWh/yr of hydrogen.

The biomass to hydrogen value chain is valuable in all of the scenarios due to the negative CO_2 emissions that it provides, and therefore in most scenarios the total biomass utilisation is close to its maximum availability in the final decade. Other biomass value chains, such as for electricity and heat, were beyond the scope of this hydrogen-focussed study but may be more favourable than the biomass-to-hydrogen value chain considered here.

A lower COP of 2 for both domestic and commercial electric heat pumps had a limited effect on the results in Figure 6-6. For more details, see the supplementary material[††].

The cost effectiveness of the different policies can also be compared. Figure 6-8 shows the total hydrogen production across all decades for each scenario, plotted against the overall system cost. The overall system cost is measured relative to the "steady" CO_2 budgets case, thus showing the additional cost to the system of the hydrogen intervention. These cost results assume that policies are revenue-neutral: for example, the payments made by the government for FITs or capital grants would be recouped elsewhere, e.g. through taxation. Therefore increases in system cost are not affected by the financial value of the policy intervention but only by its influence on the overall system behaviour.

As Figure 6-8 shows, hydrogen injection obligations and FITs both show a similar relationship between the increase in overall hydrogen usage and the impact on overall system costs. However, this policy cost-effectiveness, as defined in Equation 6.8, shows some variation depending on policy type and magnitude.

Capital grants are clearly the least cost-effective incentive. The 50% capital grant has a negligible impact on hydrogen usage, whilst increasing system costs by £4.5bn compared to the case with no hydrogen incentives. The 100% capital grant is marginally more effective, but the hydrogen policy cost-effectiveness is over £100/MWh.

Figure 6-8 shows that the hydrogen policy cost-effectiveness is quite consistent for the hydrogen injection obligations. In the "low" obligation case, with a minimum injection of 100 TWh/yr in 2050-2060, the increase in system cost is equal to £11 for each additional MWh of hydrogen production; this value rises to £14/MWh in Case 3 (with 300 TWh/yr of injection in 2050-2060). With a lower overall level of hydrogen

[††] In this thesis, see Appendix D.

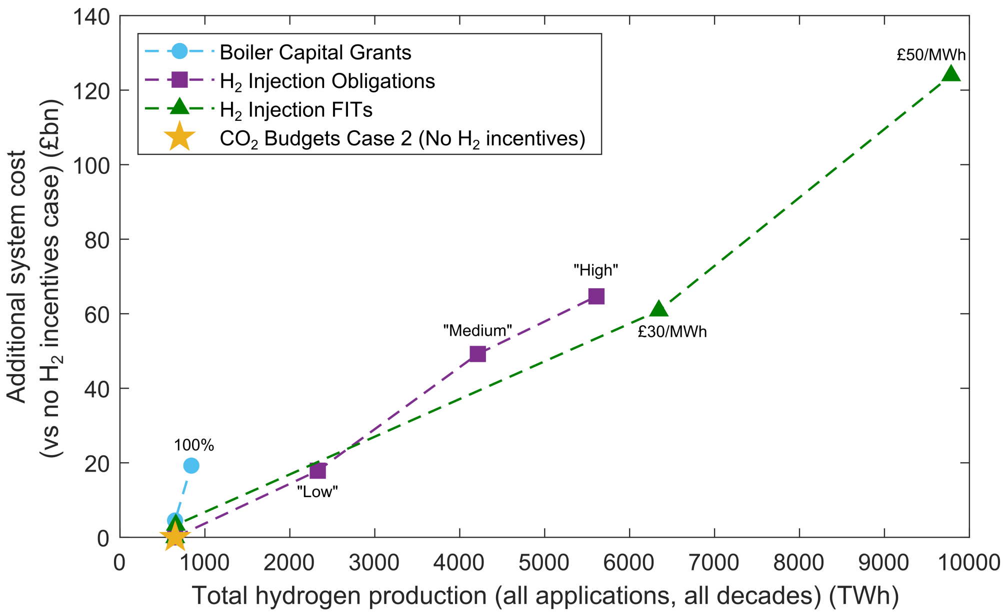

Figure 6-8: **Total hydrogen production and overall system cost in scenarios with different hydrogen incentives.** Total hydrogen production is for all applications, including industrial, commercial, and domestic demands. Overall system cost is the net present (discounted) value and is measured relative to the case with no hydrogen incentives (CO_2 Budgets Case 2).

in the system, the most cost-effective applications are used first (for example, only gas grids local to hydrogen production plants are converted); as the overall hydrogen injection requirement rises, more of the gas grid will be converted to hydrogen, but potentially in regions where the cost difference between hydrogen and the alternative (e.g. electrification) is greater.

As was shown in Figure 6-6, FITs of £10/MWh have a negligible effect on hydrogen uptake. However, FITs of £30/MWh are quite cost-effective, increasing overall hydrogen uptake at a system cost of £11/MWh. In the £50/MWh case, the cost-effectiveness falls to £14/MWh, as larger FITs incentivise hydrogen injection in locations with a greater cost difference to the alternative. The total magnitude of FIT payments in the final decade is £5bn/yr in the £30/MWh case and £13bn/yr in the £50/MWh case (un-discounted values).

Each of the scenarios in this section was constrained by the same CO_2 budgets and therefore has the same pathway of CO_2 emissions throughout its time horizon. Therefore the average CO_2 costs in these scenarios are driven by the additional overall system costs shown in Figure 6-8. The scenarios with lower levels of intervention, such as the "low" injection obligations case, have an average CO_2 cost of around £44/tCO_2; the scenarios with moderate intervention, including the "medium" and "high" injection obligations cases and the £30/MWh FIT case, have average CO_2 costs of £54–58/tCO_2; finally the £50/MWh case has an average CO_2 cost of £76/tCO_2.

6.4.3 Consumer costs

Overall system costs are useful for comparing the relative costs of different decarbonisation pathways but in reality, it is likely that any energy policy costs will be borne by the consumer. Therefore, it is also valuable to calculate and compare consumer costs. Figure 6-9 presents estimates for annual consumer heating bills for three different heating scenarios. Details on how these bills were calculated are given in Section 6.3.4.5.

As can be seen from Figure 6-9, electrification results in lower overall consumer heating bills than hydrogen. The annual electrification bill is £715/yr, which is 10% greater than a typical present-day natural gas bill (£708/yr, based on 15 MWh/yr); meanwhile the hydrogen bill is £1070/yr, which is 51% higher than the natural gas benchmark.

In the electrification scenario, the energy costs are relatively low, at only £18 per MWh of heat consumed. There are two reasons for this. First, the cost of electricity

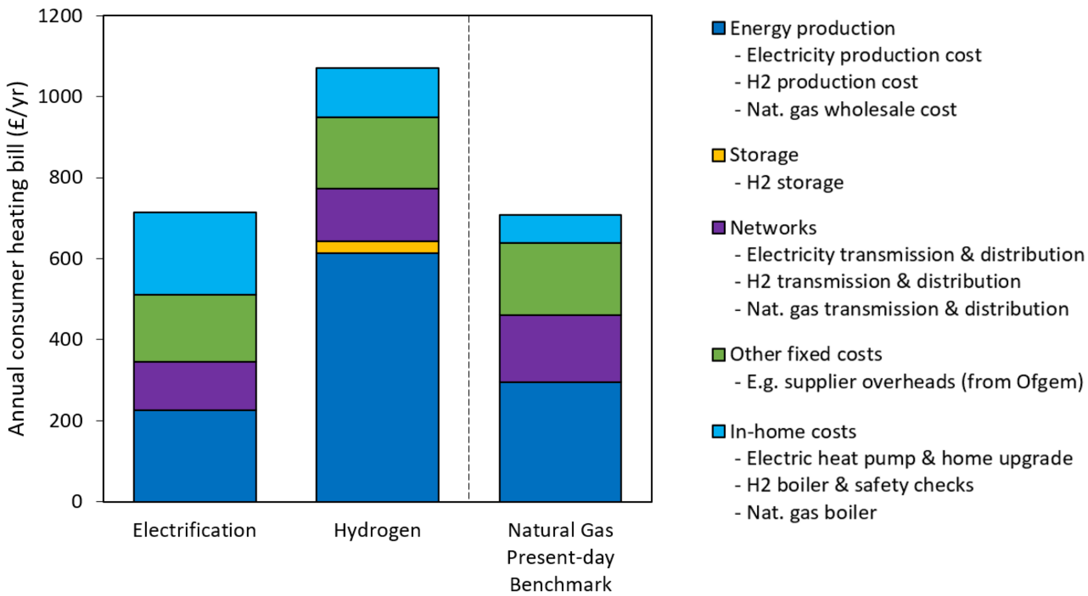

Figure 6-9: **Annual consumer heating costs for three different heating scenarios.** The electrification scenario is based on a domestic electric heat pump and is calculated from the results of the "steady" CO_2 budgets case. The hydrogen scenario is based on conversion of gas grids to hydrogen and is taken from the "high" hydrogen injection obligations case. Finally, a typical present-day natural gas bill for a UK consumer is presented for comparison [85, 86].

production in the final decade of the optimised electrification scenario is relatively low, at approximately £43/MWh. This is the average cost for the entire energy mix (as shown in Figure 6-5), including the natural gas and hydrogen peaking plants. Second, heat pumps require much less energy input to produce 1 MWh of heat than using a hydrogen boiler. The annual electricity consumption for this bill was 5.1 MWh/yr, which is the average consumption for a household with a heat pump in the scenario results.

Infrastructure costs (including transmission and distribution) are also relatively low in the electrification scenario, despite the fact that electricity infrastructure is relatively expensive on a per-capacity basis [73]. This is also partly due to the heat pump coefficient of performance: for each 1 MWh of heat delivered, only 0.4 MWh of electricity must be distributed. Furthermore, in the electrification scenario, electricity infrastructure is used to deliver both heat and non-heat electricity demands. This has two benefits: the infrastructure costs are shared across a larger total energy demand; and the non-heat demands are less variable, so the overall utilisation factor for the electricity infrastructure is higher, resulting in a lower infrastructure cost per MWh of capacity.

Finally, the in-home costs associated with electrification, including installation of a heat pump and any further home upgrades, such as installing new radiators, are a significant contributor to the annual cost to the consumer. Although these are larger than in the other cases, they are offset by the other cost components being cheaper. The equivalent consumer heating bill was also calculated for the heat pump sensitivity case, with a COP of 2, and the annual bill was found to be £863/yr: 21% greater than the electrification scenario with a COP of 2.5, but still 19% lower than the hydrogen scenario.

As Figure 6-9 shows, the annual heating bill in the hydrogen scenario is dominated by the energy costs of the hydrogen itself. The cost of the hydrogen production was based on SMR with CCS, with an average cost of £44/MWh, driven primarily by a natural gas price of £24/MWh and the costs of the SMR + CCS installations. SMR with CCS contributes 81% of hydrogen production in the scenario results: the costs of hydrogen from bioenergy and power-to-gas were not included, as these value chains have wider system interactions that are harder to account for. For example, the average bioenergy hydrogen cost in the scenario is around £126/MWh, but this does not account for the negative emissions benefits of this value chain. Meanwhile power-to-gas primarily uses excess electricity with an uncertain price: assuming that the electricity is zero-cost, the average power-to-gas hydrogen cost is around £19/MWh.

Compared to the electrification scenario, the hydrogen scenario does not benefit from an apparent efficiency of more than 1, so the final contribution of hydrogen costs to the heating bill is £48 per MWh of heat (compared with £18/MWh for the electricity scenario). The annual hydrogen consumption for this bill was 13.9 MWh/yr, which is the average consumption for a household with a hydrogen boiler in the scenario results. This value is lower than the benchmark present-day natural gas consumption of 15 MWh/yr, mainly due to projected improvements in household thermal performance between now and 2050.

The costs of the distribution infrastructure in the hydrogen case are very similar to the costs in the present-day natural gas bill and are driven by the fixed operating costs of the networks. The investment costs arising from converting natural gas grids to hydrogen, assumed to be £3500 per MW of grid capacity [73], contribute only £1.60 to the annual consumer heating bill.

Therefore, despite the relatively high costs of installing an electric heat pump, the electrification scenario is cheaper than the hydrogen scenario overall. Between the three options shown in Figure 6-9, most cost components are very similar. However, the high energy costs for hydrogen result in a significantly higher annual cost in this scenario. These results also highlight the limited effectiveness of capital grants, for either the conversion of distribution grids to hydrogen or the installation of hydrogen boilers in homes, as neither of these is sufficient to reduce the consumer cost to less than the equivalent cost of electrification.

It may be possible for hydrogen to be produced more cheaply, for example through power-to-gas with low-cost electricity. However, the results presented in Figure 6-9 represent the optimal supply chain identified in this study for delivering 300 TWh/yr of hydrogen to the gas grid. At this scale, SMR is the lowest-cost option. The results in this study suggest that the capacity for low-cost power-to-gas is limited, due to a limited availability of low-cost electricity, and competing electricity demands. For example, in all of the scenarios with various hydrogen incentives presented in Figure 6-6, the largest contribution of power-to-gas is 25 TWh/yr.

6.5 Conclusions

This study has assessed policies for decarbonising energy and incentivising emerging energy technologies, in particular hydrogen. First, a range of energy and decarbonisation policies were reviewed and their applicability to hydrogen was considered. An energy value chain optimisation model, the Value Web Model, was then applied to a representative national energy system to quantify the effects of different policies on the pathway to a net-zero energy system and the role of hydrogen within the system. This is the first time that a detailed spatio-temporal value chain optimisation model has been used to evaluate the relative effectiveness of energy policies.

Transitions to net-zero using both CO_2 budgets and CO_2 taxation were modelled. Whilst either approach is capable of achieving net-zero emissions, differences were identified in overall system cost and decarbonisation trajectory. The decarbonisation trajectory can have a significant impact on costs, overall emissions, and energy system behaviour. The practicalities of implementing these policies are difficult to model but may be important: for example, whether it is possible to include all system emissions within a CO_2 budget or taxation system. CO_2 prices depend on the pricing policy that is implemented (for example, taxation or trading) but may need to be in excess of £300/tCO_2 in 2050 in order to achieve net-zero emissions.

It was found that earlier decarbonisation trajectories would result in a slightly more expensive energy transition. However, these trajectories also result in significantly lower total emissions over the entire time horizon, and therefore the cost per tonne of CO_2 saved is lower overall. Earlier decarbonisation may also be beneficial in a carbon cap-and-trade scheme, as costs are spread over a longer time period and the final CO_2 trading price may be lower. Hydrogen was found to have a role in the optimised net-zero energy system but this was mostly limited to providing industrial heat. Therefore, further scenarios with additional policies to support hydrogen technologies were studied. Obligations and feed-in tariffs for injection of hydrogen into gas grids were found to be similarly effective for incentivising hydrogen technologies. In either case, overall system costs were increased at a rate of £11–14 per additional MWh of hydrogen used over the four decade time horizon. Capital grants for hydrogen boilers, however, were not found to influence the optimal decarbonisation pathway.

Steam methane reforming (with CO_2 capture and storage) was found to be the preferred hydrogen production method in all scenarios with a significant level of hydrogen uptake. Both power-to-gas and biomass gasification were found to make contributions and are valuable for providing system flexibility and negative CO_2 emissions, respectively. However, the contribution that either value chain can make to large scale hydrogen production may be limited: for power-to-gas, there is a limited availability of low-cost electricity, especially with competing electricity demands; for bioenergy, it is essential that only sustainable biomass sources are used, and there could be preferred uses for the biomass, such as electricity production.

Considering the costs of conversion of gas grids to hydrogen, it was found that consumer heating bills may be 50% larger when using hydrogen for heating than when using an electric heat pump. This cost difference is driven by energy costs; infrastructure costs for the two heating value chains were found to be similar.

The optimisation scenario results presented in this study provide insights into the optimal pathways to reach net-zero and the potential effects of different policy interventions on the energy system. However, challenges still exist in converting optimisation results into real-life policy actions. For example, in this study CO_2 budgets were found to be the most efficient way of ensuring that a net-zero system is achieved by 2050. However, this assumes that all emissions across the system can be tracked and controlled, which would be challenging to do in practice. Carbon cap-and-trade and similar schemes can assist with this, but in reality it is likely that a range of sector-specific regulations will be needed. A further example is where technologies provide valuable services that are not necessarily rewarded by conventional energy markets. In this study, hydrogen was found to have a valuable role in providing system flexibility, with both underground and pressure vessel hydrogen storage being used in the net-zero energy system. Through optimisation, it is clear to see that including these technologies reduces the overall system costs. However, in reality, it is important that these flexibility services are valued, for example through specific support of the technologies or creation of flexibility markets.

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Article appendices

The article version of this chapter, as submitted to Sustainable Production and Consumption, includes appendices with abbreviations and the model nomenclature. In this thesis, the abbreviations can instead be found at the beginning of the article, and the full model nomenclature is provided in Appendix A of the thesis. The full article supplementary material is not provided with this thesis, however details of the input data are provided in Appendix B of this thesis, and details of the sensitivity scenarios that were modelled are given in Appendix D.

Chapter concluding remarks

The article that has been presented in this chapter is the final study that was performed as part of this thesis. It uses the modelling methodology that was developed over the previous chapters, applying it to the most comprehensive set of scenarios presented in this thesis. The scenarios give insights into the role of hydrogen within decarbonising energy systems and the impact of different policy interventions on the energy transition.

The modelling methodology in this chapter was largely unchanged from previous chapters, however a new set of scenarios were modelled with a comprehensive representation of hydrogen value chains within Great Britain. Notably, the scenarios in this study include a four decade time horizon, so that the transition from the present day system to a decarbonised 2050 system could be modelled. In particular, the development of costs and emissions across the time horizon could be studied, understanding the consequences of early or late action. The other significant addition in this study was the inclusion of bioenergy value chains, in particular because this enabled the modelling of "negative emissions", and therefore "net-zero" as a decarbonisation target.

The results in this chapter follow similar trends to the previous studies, including a significant expansion of electricity value chains, and in general a preference for electrification, for example in domestic heating. Where opportunities arise for hydrogen without specific incentives, they are predominantly in industry, or for energy system flexibility. The preferred large-scale hydrogen production value chain is steam methane reforming, but power-to-gas is also valuable when it can access low-cost electricity.

Despite being a relatively expensive value chain, hydrogen from biomass also appears to be valuable to the energy system, in particular because it provides negative CO_2 emissions. In the scenarios presented in this chapter, biomass usage was at the maximum that was allowed by the model constraints, reaching 64 TWh of primary biomass energy per year in 2050. Whether bioenergy value chains make a significant contribution to future energy systems will depend on the availability of biomass supply, and the capability for these value chains to actually achieve negative emissions. The issues around bioenergy value chains are complex, and beyond the scope of this thesis.

Insights were also gained in this study regarding the impacts of different policy interventions on the overall system and the individual consumer. Whilst optimisation studies may be performed that consider overall "system cost", it is important to consider who will actually pay these costs in practice. The results in this chapter suggest that a hydrogen for heating decarbonisation pathway could result in significantly higher consumer bills than an alternative pathway based on electric heat pumps.

Chapter 7

Conclusion

In this thesis, value chain optimisation has been used to explore the role of hydrogen in future energy systems. In this chapter, conclusions from the research are provided, followed by recommendations for future work and for innovation and policy.

7.1 Research conclusions

The aims of this thesis were: to understand energy systems and hydrogen; to design and model scenarios; and to interpret the model results to provide insights into the role of hydrogen in energy systems. In the following subsections, the findings with respect to each of these aims will be summarised.

7.1.1 Understand energy systems and hydrogen

Throughout this thesis, an understanding of existing energy systems and the challenges of the energy transition has been established. A comprehensive dataset has been developed that includes data for a wide range of technologies and resources in the Great Britain energy system (and is included as an appendix to this thesis). Furthermore, the design and operation of the natural gas transmission and distribution system was explored. As was shown in Chapter 5, this natural gas infrastructure plays an essential role in the present-day energy system, as it both transports and distributes energy and provides energy system flexibility through its linepack. Furthermore, the gas grid could also be a key component of future hydrogen systems.

Many of the aspects of hydrogen as an energy carrier have been explored in this thesis. The concept of power-to-gas was introduced and its practicalities were explored, including a study of real-life power-to-gas projects worldwide. The practicalities of injecting hydrogen into gas grids were considered. It was shown that under the same operating conditions, a pipeline carrying hydrogen may have an energy throughput that is 30% lower than if the pipeline carried methane, whilst the linepack flexibility could be reduced by as much as 80%. Data was acquired for a range of technologies within hydrogen value chains, including all of the key hydrogen production pathways. This data includes costs and operating parameters for both the present day and future decades.

Other emerging energy technologies have also been considered in this thesis. CO_2 value chains were considered in detail, including the practicalities, costs, and energy and environmental impacts of CO_2 capture, utilisation and storage technologies. The prospect of achieving negative emissions by using bioenergy with CO_2 capture and storage was also considered.

7.1.2 Design and model hydrogen scenarios

By studying previous modelling work and the characteristics of hydrogen as an energy carrier, this thesis has explored the key requirements for modelling hydrogen in energy systems. In Chapter 2, previous modelling studies of power-to-gas were reviewed, and it was found that most studies either focussed on specific business cases, or used broad energy models that lacked the details to model the specific business cases that may be available to power-to-gas. This trend was continued in Chapter 3, where it was argued that the modelling approaches and scenarios used in influential global energy studies lack the spatial, temporal and technological details to model the subtle contributions that hydrogen could have in energy systems, such as absorbing excess electricity or providing sector coupling. A series of recommendations for developing energy scenarios were established, such as using modelling tools with sufficient detail, including the right sectors and technologies, making realistic data assumptions, and having an appropriate level of ambition.

This thesis has shown the strengths of a value chain optimisation approach for modelling changing energy systems, and the role of hydrogen in particular. Value chain optimisation can include a detailed representation of technologies, both in terms of the variety of technologies that are modelled, and the detail with which each technology is modelled. For example, the operation of each individual technology can be realistically represented. Furthermore, value chain optimisation tracks resource flows from primary resource to end use, ensuring realistic energy system operation. This can differ from many large-scale energy models, which may ensure overall energy equilibrium, but lack more detailed information on technology operation and resource transmission, distribution and storage.

In this thesis, the Value Web Model was used to model hydrogen value chains within the wider energy system. The Value Web Model is well suited to this task, as it can represent a wide variety of energy value chains, including hydrogen value chains and others. Importantly, the Value Web Model also models the interconnectivity of different value chains, including between different sectors. Furthermore, the model includes representation of energy transportation and storage. All of these aspects are essential for accurate representation of hydrogen within energy systems.

Throughout this thesis, the Value Web Model has been configured, and scenarios have been developed, in order to represent hydrogen and the wider energy system in more depth. New model configurations include a new representation of CO_2 value chains, enabling the representation of CO_2 as a resource to be used by different technologies including CO_2 utilisation and storage. This was the first time that CO_2 value chains had been incorporated into value chain optimisation in this way. A more detailed representation of natural gas grids was also included as part of this thesis. Linepack storage capacity was incorporated into transmission pipelines, meaning that both their transportation and storage capacity was included. Distribution systems were also modelled, so that the costs and operating requirements of these networks were included, again with linepack capacity being modelled. Finally, hydrogen injection into gas grids was modelled, including options for partial injection in existing gas grids, and the complete switch-over from natural gas to hydrogen.

As part of the scenario development, a comprehensive dataset was generated, using a range of methods including literature review, GIS analysis and processing of temporal data. As well as providing the model input data for this thesis, this extensive dataset is also valuable to other energy researchers. The data has been published in a Data-in-Brief article, and is reproduced in Appendix B of this thesis. Finally, the scenarios were designed with a variety of technology, economic and policy assumptions, to represent issues for the Great Britain energy system as it transitions to a low-carbon system in 2050.

7.1.3 Interpret model results to provide hydrogen insights

The value chain modelling was used to generate insights about the role of hydrogen and other value chains in decarbonisation. Each of chapters 4 to 6 gave specific conclusions based on the scenarios that were modelled. It is also possible to draw broader conclusions about the role of hydrogen from the trends from these studies.

In Chapter 4, it was found that CO_2 capture and utilisation may be able to produce some products at prices competitive in existing markets, but that the scope for these value chains to provide reductions in overall emissions was small. CO_2 capture and storage was also found to have a limited role in decarbonising the domestic sector, with uptake of renewables and electrification preferred. However, only the domestic sector was considered in this chapter, so there may be a greater role for CO_2 storage in other sectors.

In Chapter 5, it was found that partial hydrogen injection into existing natural gas grids is viable now, with feed-in tariffs in the range of £20-50/MWh sufficient to incentivise it in the present-day system. Achieving higher levels of partial injection becomes increasingly expensive, due to the need for additional hydrogen storage or production infrastructure to follow the variable demands of gas in the grid. Whether complete conversion of gas grids to hydrogen is the most cost-effective option depends on the costs and challenges associated with the main alternative, which is electrification.

Finally, in Chapter 6, it was found that hydrogen has a role in the optimal net-zero energy system without any additional incentives. However, this role is largely supplementary, providing flexibility to the wider energy system. As in Chapter 5, hydrogen only begins to have a more significant role in direct energy supply when other technologies, such as electric heat pumps, are not available. Chapter 6 also considered the use of bioenergy for hydrogen production, and found that this value chain is valuable when combined with CO_2 capture and storage as it can deliver negative emissions. However, any potential bioenergy value chains need to be considered carefully to ensure that they are truly sustainable, and other possible value chains for bioenergy should also be considered, such as conversion to electricity.

More broadly, the results from this thesis suggest that hydrogen can have a valuable role in aiding energy system decarbonisation, but that it cannot be expected to solve all decarbonisation challenges.

In many contexts, hydrogen is relatively expensive to produce, and therefore is unlikely to be able to compete with alternative energy carriers on the basis of cost alone. Hydrogen production requires another energy feedstock and a conversion step that is both expensive in itself and has energy losses. As a result, hydrogen is unlikely to be cheaper than the energy feedstocks it requires, such as natural gas or electricity.

Nonetheless, hydrogen has non-cost advantages that could make it a valuable energy carrier. Compared to electricity, hydrogen can be stored much more easily at large scales, for example using underground storage. Consequently, there are flexibility benefits to energy systems, such as helping to balance supplies and demands of electricity. Meanwhile compared to fossil fuels, hydrogen offers comparable energy density but with potentially lower or zero CO_2 emissions. As was identified in this thesis, this makes hydrogen an appealing option for industrial decarbonisation, but there are also other potential sectors, such as transport, aviation and shipping. Provided that energy systems appropriately value these flexibility and decarbonisation benefits (for example using the policies considered in Chapter 6), hydrogen can become a competitive energy carrier.

Multiple hydrogen production options exist, each with different advantages. For large-scale applications, this thesis identified natural gas reforming with CCS to be the most suitable hydrogen supply chain. This is because natural gas reforming can offer a large-scale, reliable, low-cost supply of hydrogen. However, CO_2 capture and storage facilities will be required for this supply chain to deliver low-carbon hydrogen. It will be possible to produce hydrogen at low cost from excess electricity, especially as electrolyser costs fall in future decades, however the scale of production from this route may be limited. Electrolyser plant sizes will be required to scale up significantly, and there will also be a limit to the availability of low-cost electricity, especially with competing new demands for electricity. Bioenergy value chains could also contribute, but are also unlikely to deliver large-scale hydrogen supply due to limited biomass availability and competing demands.

For hydrogen to become established within the energy system and begin delivering wider system benefits, the best strategy is likely to be to establish it in applications where it has potential at scale, such as in industry. Developing these supply chains will incentivise the installation of hydrogen transportation and storage infrastructures, which will make it easier for hydrogen to provide flexibility services such as dispatchable power generation. Without the consistent large-scale hydrogen demand, using hydrogen for flexibility would be much more expensive as the necessary infrastructures would have lower utilisation over the course of the year.

Partial injection of hydrogen into gas grids may be appealing for the same reasons. Preparing gas grids for partial injection is relatively inexpensive, and the cost of hydrogen would have a small impact on consumer energy bills. However, with a consistent hydrogen demand, it will be easier for hydrogen supply chains to establish themselves. However, the decarbonisation potential of partial hydrogen injection is limited. Full decarbonisation of heating through hydrogen would require conversion of gas grids to hydrogen, but this would have a much greater impact on consumer energy bills, due to the high costs of hydrogen production. The hydrogen production costs are likely to outweigh any energy transportation and distribution costs, therefore the "sunk costs" of natural gas grids are not a sufficient justification for converting them to hydrogen. The modelling in this thesis suggests that electrification of heating is likely to be a lower cost option in Great Britain, provided that electric heat pumps can be rolled out to the majority of homes.

7.2 Recommendations

7.2.1 Recommendations for further research

Energy systems modelling can be highly valuable for providing information on optimal future pathways for energy systems, and hence informing policy and investment decisions. Continued modelling is required as our understanding of emerging energy technologies develops. Most importantly, future modelling work should be careful to adhere to the recommendations that were set out in Chapter 3, including sufficient spatial, temporal and technological detail, and modelling transparency.

Value chain optimisation is a valuable tool for modelling energy systems, and should be continued. There are a number of areas where depth and breadth could be added to the modelling of energy systems in this thesis. A larger model scope enables more interactions between value chains, identifying yet more potential synergies and opportunities for sector-coupling. Adding the transport sector to the model scope in this thesis would enable the comparison of hydrogen and electricity as low-carbon supply chains for transport, and as well as assessing the potential for electric vehicles to provide energy system flexibility. A richer representation of heat could also be included, for example including electric storage heaters and hybrid heat pumps. Finally, even more components of hydrogen value chains could be added, such as alternative hydrogen storage and transportation technologies, and use of hydrogen as a chemical feedstock.

Greater spatial and temporal detail in modelling may also illuminate further opportunities for energy systems. Furthermore, probabilistic methods would enable a greater consideration of the variability of renewable energy sources and energy demands. However, improving modelling detail, whether in terms of model scope or functionality, has a trade-off with computational demand. Improving computational power may help with modelling more complex scenarios in the future.

7.2.2 Recommendations for innovation and policy

The results from this thesis show that hydrogen has value for aiding energy decarbonisation, especially in a flexibility role. Furthermore, provided that sufficient policies are in place to incentivise emissions reductions, hydrogen should not require any additional incentives in order to establish itself in energy systems. Instead, opportunities for hydrogen to provide flexibility will arise unaided. However, in many sectors decarbonisation will only occur if policies are put in place to ensure that low-carbon options are preferred to fossil fuels (without CO_2 capture). Various options exist for this, including direct regulation and CO_2 pricing.

Nonetheless, there is a role for innovation investment to ensure that the necessary hydrogen technologies reach their full potential. Electrolysis will be a key technology in many future hydrogen value chains. Electrolyser costs are projected to fall significantly in future decades, but only if production is scaled up. This scale-up looks promising based on the numerous new large-scale (larger than 10 MW) projects that have been announced, however there is a role for governments in ensuring that these projects are actually realised.

Likewise, CO_2 capture and storage is an essential technology in many low-carbon energy value chains, including hydrogen. CO_2 storage has been demonstrated in various locations globally, but from a UK perspective it is key that a facility is demonstrated as soon as possible, given the reliance of many decarbonisation pathways on this technology.

Finally, hydrogen can have a strong role in helping to decarbonise industry. Therefore innovation spending should be used to ensure that technologies are developed and commercialised that can replace the incumbent fossil fuel based technologies in this sector. Opportunities for hydrogen in industry include in refining, steel production and various heating applications.

Although policies that support hydrogen directly should not be essential for hydrogen to emerge in energy systems, there are some policies that could help to accelerate the transition. Partial hydrogen injection into gas grids is an opportunity to establish a demand for hydrogen and achieve some reduction in emissions. There is an increasingly strong evidence base that partial injection up to level of around 20 vol.% is practical and safe, so governments should be ready to legalise this level of injection. Optionally, further incentives for hydrogen injection could be used, such as feed-in tariffs, however as was shown in Chapter 5, these incentives are not especially efficient for decarbonisation.

Low-carbon hydrogen in industry could also be incentivised, both for the energy uses that were described above, and in applications where hydrogen is already used. For example, the largest use of hydrogen currently is as a chemical feedstock, but this hydrogen is almost always produced from fossil fuels without CO_2 capture. Incentives to decarbonise industry could include price support such as feed-in tariffs, or an obligation scheme for a minimum level of low- or zero-carbon hydrogen used, or a maximum allowable CO_2 intensity for the chemical product.

Finally, policymakers should be cautious with incentives for large-scale uptake of hydrogen in other sectors, such as domestic heating. The large extent and reliance on natural gas grids in countries like the UK may make large-scale conversion of these assets to hydrogen appear to be a more straightforward option than electrification. However, due to the cost of hydrogen production, this choice may prove more expensive than alternatives in the long run. A decision to convert large portions of the gas grid to hydrogen should only be made if it can be shown that electrification would be impractical or prohibitively expensive.

Appendices

Contents

Appendix A

Value Web Model nomenclature

This appendix provides a complete nomenclature for the Value Web Model, including for the constraints presented in this thesis. The complete Value Web Model formulation for the model prior to the work of this thesis is documented in publications by Samsatli and co-workers [1, 2, 3].

As the majority of the resources that were modelled are energy vectors, the most convenient unit for quantities of these resources is MWh and for flows of these resources is MW (MWh/h). However, these units may not be appropriate for all resources in a value web. For example, in this thesis, the units used for CO_2 are t and t/h (tonnes and tonnes per hour). In the following nomenclature section, the units for each resource are indicated by the unit "UoR", for "unit of resource", which stands for the relevant unit for that resource: e.g. MWh for most energy resources, t for CO_2, and so on. The rates of operation of conversion technologies are all in MW, since most are concerned with the production of energy vectors. The units of the conversion factors convert from operation in MW to production of each resource in its own units: thus the units of the conversion factors are (UoR/h)/MW.

Indices and sets

$b \in \mathbb{B}$	Transport infrastructures
$c \in \mathbb{C} \subset \mathbb{R}$	Biomass resources (“crops”)
$d \in \mathbb{D}$	Daily interval types (e.g. weekday, weekend)
$\mathbb{E} \subset \mathbb{R}$	End vectors
$f \in \mathbb{F}$	Transportation direction of flow
$i \in \mathbb{I}$	System impacts (e.g. costs, CO_2 emissions)
$h \in \mathbb{H}$	Hourly intervals
$l \in \mathbb{L}$	Linepack technologies
$m \in \mathbb{M}$	Transport technologies
$p \in \mathbb{P}$	Conversion technologies
$\mathbb{P}^{\mathrm{D}} \subseteq \mathbb{P}$	Domestic conversion technologies
$\mathbb{P}^{\mathrm{C}} \subseteq \mathbb{P}$	Commercial/industrial conversion technologies
$\mathbb{P}^{\mathrm{HIGG}} \subseteq \mathbb{P}^{\mathrm{C}}$	Conversion technologies relating to partial hydrogen injection
$\mathbb{P}^{\mathrm{Dist}} \subseteq \mathbb{P}^{\mathrm{C}}$	Gas distribution conversion technologies (including natural gas and hydrogen)
$r \in \mathbb{R}$	Resources
$s \in \mathbb{S}$	Storage facilities
$\mathbb{S}^{\mathrm{Dist}} \subseteq \mathbb{S}$	Gas distribution storage technologies (representing gas grid linepack)
$sl \in \mathbb{SL}$	Solar PV installation types (e.g. solar farm and rooftop)
$t \in \mathbb{T}$	Seasonal time intervals
$w \in \mathbb{W}$	Wind turbine type (e.g. onshore and offshore)
$y \in \mathbb{Y}$	Long term planning time intervals (e.g. decadal)
$\tilde{y} \in \tilde{\mathbb{Y}}$	Yearly intervals used for discounting costs
$z \in \mathbb{Z}$	Spatial zones

Parameters

$A^{\mathrm{W,max}}_{wzy}$	Total area of land available for wind turbine type w in zone z in planning period y [m^2]
$A^{\mathrm{Sl,max}}_{slzy}$	Total area of land available for solar PV installation type sl in zone z in planning period y [m^2]

$A^{\mathrm{Bio,max}}_{zy}$	Total area of land available for growing biomass in zone z in planning period y [ha]
a_{lz}	Binary value determining whether there is availability to build a connection (pipeline) to linepack system l in zone z ($a_{lz} = 1$ if a connection may be built, 0 otherwise)
a_{sz}	Binary value determining whether there is availability for a storage facility s in zone z ($a_{sz} = 1$ if a facility may be built, 0 otherwise)
BR_{py}	Total allowable number of conversion technologies p that may be built in planning period y (build rate)
b^{max}_{b}	Maximum flow rate of transport infrastructure b [UoR/h]
C^{B}_{biy}	System impact of the capital investment in a length of transport infrastructure b in planning period y [£/(connection-km) or tCO_2/(connection-km)]
C^{P}_{piy}	System impact of the capital investment in a conversion technology p in planning period y [£ or tCO_2]
C^{S}_{siy}	System impact of the capital investment in a storage facility s in planning period y [£ or tCO_2]
C^{L}_{liy}	System impact of the capital investment in a connection to linepack system l in planning period y [£ or tCO_2]
C^{W}_{wiy}	System impact of the capital investment in wind turbine type w in planning period y [£ or tCO_2]
C^{Sl}_{sliy}	System impact of the capital investment in solar PV installation type sl in planning period y [£ or tCO_2]
c^{Bio}_{city}	System impact of producing a unit of biomass crop c in season t of planning period y [£/UoR or tCO_2/UoR] (impacts of planting, cultivating and harvesting the crop)
c^{M}_{rihdty}	System impact of importing a unit of resource r during hour h, day type d, season t and planning period y [£/UoR or tCO_2/UoR]
c^{U}_{rihdty}	System impact of producing a unit of resource r during hour h, day type d, season t and planning period y (e.g. domestic natural gas production) [£/UoR or tCO_2/UoR]
c^{X}_{rihdty}	System impact of exporting a unit of resource r during hour h, day type d, season t and planning period y [£/UoR or tCO_2/UoR]

$D^{\mathrm{C}}_{\star iy}$	Factor for discounting capital investments made in planning period y back to the beginning of the time horizon (i.e. the start of the first planning period). $\star$ represents transport infrastructures b , conversion technologies p, storage technologies s or linepack technologies l.
D^{OM}_{iy}	Factor for discounting O&M impacts incurred in planning period y back to the beginning of the time horizon
D^{W}_{wiy}	Factor for discounting capital investments in new wind turbines made in planning period y back to the beginning of the time horizon
D^{Sl}_{iy}	Factor for discounting capital investments in new solar PV installations made in planning period y back to the beginning of the time horizon
$D^{\mathrm{act}}_{rzhdty}$	Demand for resource r in zone z during hour h, day type d, season t and planning period y [UoR/h]
$D^{\mathrm{comp}}_{rzhdty}$	Compulsory demand (that must always be satisfied) for resource r in zone z during hour h, day type d, season t and planning period y [UoR/h]
$D^{\mathrm{opt}}_{rzhdty}$	Optional demand (that may be satisfied if there are system benefits, e.g. revenues) for resource r in zone z during hour h, day type d, season t and yearly period y [UoR/h]
$d_{zz'}$	Distance between the centres (demand-weighted) of spatial zones z and z' [km]
f^{loc}_{zy}	Maximum allowable fraction of suitable biomass growing area in zone z that may be used in planning period y
f^{nat}_{y}	Maximum allowable fraction of suitable biomass growing area across the entire country that may be used in planning period y
$l^{\mathrm{get,max}}_{l}$	Maximum withdrawal rate from a linepack system l via a single connection (pipeline) [UoR/h]
$l^{\mathrm{put,max}}_{l}$	Maximum injection rate into a linepack system l via a single connection (pipeline) [UoR/h]
$l^{\mathrm{hold,max}}_{l}$	Maximum storage inventory represented by each single connection (pipeline) of linepack system l [UoR]
$l^{\mathrm{hold,min}}_{l}$	Minimum storage inventory represented by each single connection (pipeline) of linepack system l [UoR]
MB_{mb}	Binary value that determines whether transport technology l can use infrastructure b, (= 1 if it can, 0 otherwise)

$m^{\max}_{rzhdty}$	Maximum allowable import rate of resource r in zone z during hour h, day type d, season t and planning period y [UoR/h]
n^{hd}_{h}	Duration of hourly interval h [h]
n^{dw}_{d}	Number of occurrences of day type d in a week (e.g. 5 for a weekday, 2 for a weekend)
n^{wt}_{t}	Number of repeated weeks in season t
n^{yy}_{y}	Number of repeated years in planning period y
N^{ESl}_{slzy}	Number of pre-existing solar PV installations of type sl in zone z in planning period y (accounts for estimated retirement dates)
N^{EW}_{wzy}	Number of pre-existing wind turbines of type w in zone z in planning period y (accounts for estimated retirement dates)
N^{EPC}_{pz}	Number of pre-existing commercial conversion technologies of type p in zone z
NR^{EPC}_{pzy}	Number of pre-existing commercial conversion technologies of type p in zone z that retire at the beginning of planning period y
N^{ES}_{sz}	Number of pre-existing storage technologies of type s in zone z
NR^{ES}_{szy}	Number of pre-existing storage technologies of type s in zone z that retire at the beginning of planning period y
$N^{\mathrm{EB}}_{bzz'}$	Number of pre-existing transport infrastructure connections of type b between zones z and z'
N^{EL}_{lz}	Number of pre-existing linepack connections (pipelines) of type l in zone z
NR^{EL}_{lzy}	Number of pre-existing linepack connections (pipelines) of type l in zone z that retire at the beginning of planning period y
N^{house}_{zy}	Number of households in zone z in planning period y
$p^{\max}_{p}$	Maximum operating rate of technology p [MW]
$p^{\min}_{p}$	Minimum operating rate of technology p [MW]
$p^{\max}_{sl}$	Maximum operating rate of solar PV installation sl [MW]
$q^{\max}_{m}$	Maximum operating rate of transport technology l [MW]
R^{EW}_{w}	Rotor radius of pre-existing wind turbines of type w [m]
R^{W}_{w}	Rotor radius of new wind turbines of type w [m]
$RT^{\mathrm{P}}_{py'y}$	Binary value determining whether conversion technology p, invested in at the beginning of planning period y', retires at the beginning of planning period y (1 if it does retire, 0 otherwise)

$RT^{\mathrm{S}}_{sy'y}$	Binary value determining whether storage facility s, invested in at the beginning of planning period y', retires at the beginning of planning period y (1 if it does retire, 0 otherwise)
$RT^{\mathrm{L}}_{ly'y}$	Binary value determining whether a connection of linepack system l, invested in at the beginning of planning period y', retires at the beginning of planning period y (1 if it does retire, 0 otherwise)
$RT^{\mathrm{W}}_{wy'y}$	Binary value determining whether wind turbine type w, invested in at the beginning of planning period y', retires at the beginning of planning period y (1 if it does retire, 0 otherwise)
$s^{\mathrm{get,max}}_{s}$	Maximum withdrawal rate from storage facility s [UoR/h]
$s^{\mathrm{hold,max}}_{s}$	Maximum storage capacity of a single storage facility s [UoR]
$s^{\mathrm{put,max}}_{s}$	Maximum injection rate into storage facility s [UoR/h]
v^{CutIn}_{w}	Minimum operational wind speed for wind turbine [m/s]
v^{CutOut}_{w}	Maximum operational wind speed for wind turbine [m/s]
v^{Rated}_{w}	Wind speed at which wind turbine produces maximum power (rated power) [m/s]
V_{riy}	Value (e.g. price) of a unit of resource r in planning period y [£/UoR or tCO_2/UoR]
$V^{CO_2}_{y}$	The cost impact of 1 tonne of CO_2 emissions (i.e. the CO_2 price) in planning period y [£]
v_{wzhdty}	Wind speed for turbine type w in zone z during hour h of day type d in season t of planning period y [m/s]
x_z	x-coordinate of the centre of demand of spatial zone z
y_z	y-coordinate of the centre of demand of spatial zone z
Y^{Bio}_{czty}	Biomass yield potential for crop c in zone z for season t of planning period y [UoR/ha/season]
α_{rpy}	Conversion factor of resource r in technology p in planning period y
β_b	Directionality parameter for transport infrastructures b: $= -1$ if one-way unidirectional (can only be built and operated in one direction); $= 0$ if two-way unidirectional (unidirectional infrastructure but can be built in both directions); $= 1$ if bidirectional (only one infrastructure needed that can be operated in either direction)
ϵ	Weighting factor for including total energy production in objective function

γ	Finance rate
η_w	Wind turbine efficiency for wind turbine type w
ι	Discount rate
$\lambda_\star$	Economic lifetime of technologies [year] ($\star \in \{b, p, s\}$ for transport infrastructures, conversion technologies and storage technologies, respectively)
$\lambda^{\mathrm{get}}_{lrfy}$	Conversion factor for performing "get" task with linepack technology l on resource r in planning period y
$\lambda^{\mathrm{hold}}_{lrfy}$	Conversion factor for performing "hold" task with linepack technology l on resource r in planning period y
$\lambda^{\mathrm{put}}_{lrfy}$	Conversion factor for performing "put" task with linepack technology l on resource r in planning period y
$\nu_{zz'}$	Binary parameter, 1 if zone z is adjacent to zone z'
ρ^{air}	Air density [kg/m^3]
$\sigma^{\mathrm{get}}_{srfy}$	Conversion factor for performing "get" task with storage technology s on resource r in planning period y
$\sigma^{\mathrm{hold}}_{srfy}$	Conversion factor for performing "hold" task with storage technology s on resource r in planning period y
$\sigma^{\mathrm{put}}_{srfy}$	Conversion factor for performing "put" task with storage technology s on resource r in planning period y
ς	Scaling factor for impacts in the objective function. Multiplies by 10^{-6} to improve scaling in the optimisation (£ to £M and t to Mt)
$\bar{\tau}_{mrfy}$	Conversion factor for transport technology l transporting resource r in planning period y (distance-independent)
$\hat{\tau}_{mrfy}$	Conversion factor for transport technology l transporting resource r in planning period y (distance-dependent)
ϕ^{B}_{biy}	Annual O&M impact of transport infrastructure b in planning period y [(£ or tCO_2)/(connection-km-yr)]
ϕ^{P}_{piy}	Annual O&M (fixed) impact of conversion technology p in planning period y [£/yr or tCO_2/yr]
ϕ^{S}_{siy}	Annual O&M (fixed) impact of storage facility s in planning period y [£/yr or tCO_2/yr]

ϕ^{L}_{liy} Annual O&M (fixed) impact of a connection to linepack system l in planning period y [£/yr or tCO_2/yr]

ϕ^{W}_{wiy} Annual O&M (fixed) impact of wind turbines in planning period y [£/yr or tCO_2/yr]

$\phi^{\mathrm{Sl}}_{sliy}$ Annual O&M (fixed) impact of solar PV installations in planning period y [£/yr or tCO_2/yr]

$\varphi^{\mathrm{P}}_{piy}$ Variable operating impact of conversion technology p in planning period y [£/UoR or tCO_2/UoR]

$\hat{\varphi}^{\mathrm{Q}}_{miy}$ Distance-dependent variable operating impact of transport process l in planning period y [£/km/UoR or tCO_2/km/UoR]

$\bar{\varphi}^{\mathrm{Q}}_{miy}$ Distance-independent variable operating impact of transport process l in planning period y [£/UoR or tCO_2/UoR] (e.g. flat rate freight charges)

$\varphi^{\mathrm{SG}}_{siy}$ Variable operating impact of "get" task for storage facility s in planning period y [£/UoR or tCO_2/UoR]

$\varphi^{\mathrm{SH}}_{siy}$ Unit variable operating impact of "hold" task for storage facility s in planning period y [£/UoR or tCO_2/UoR]

$\varphi^{\mathrm{SP}}_{siy}$ Unit variable operating impact of "put" task for storage facility s in planning period y [£/UoR or tCO_2/UoR]

$\varphi^{\mathrm{LG}}_{liy}$ Variable operating impact of "get" task for connection to linepack system l in planning period y [£/UoR or tCO_2/UoR]

$\varphi^{\mathrm{LH}}_{liy}$ Unit variable operating impact of "hold" task for connection to linepack system l in planning period y [£/UoR or tCO_2/UoR]

$\varphi^{\mathrm{LP}}_{liy}$ Unit variable operating impact of "put" task for connection to linepack system l in planning period y [£/UoR or tCO_2/UoR]

$\chi^{\max}_{rzhdty}$ Maximum export rate of resource r in zone z in planning period y [UoR/h]

ω_i Weighting factor for including key performance indicator i in objective function

Positive variables

A^{Bio}_{czy} Area allocated to production of biomass (crop) c in zone z during planning period y [ha]

A^{Sl}_{sl} Total area occupied by solar PV installations of type sl in zone z during planning period y [m^2]

$\mathscr{C}^{\mathrm{IET}}_{zhdty}$	Amount of "capturable" CO_2 emitted in zone z during hour h of day type d in season t of planning period y [tCO_2]
$\mathscr{C}^{\mathrm{US}}_{zhdty}$	Amount of CO_2 utilised or stored in zone z during hour h of day type d in season t of planning period y [tCO_2]
$D^{\mathrm{sat}}_{rzhdty}$	Optional demands satisfied in zone z during hour h of day type d in season t of planning period y [UoR/h]
E_{rzhdty}	Excess production of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
f^{heat}_{pzy}	Fraction of heat satisfied by domestic heating technology p in zone z in planning period y
I_{szhdty}	Inventory in storage facility s in zone z during hour h of day type d in season t of planning period y [UoR]
$I^{0,\mathrm{act}}_{szdty}$	Inventory in storage facility s in zone z at the start of day type d of season t in planning period y [UoR]
$I^{0,\mathrm{sim}}_{szdty}$	Inventory in storage facility s in zone z at the start of the simulated cycle for day type d of season t in planning period y [UoR]
$\mathscr{I}^{Total}_{iy}$	Total net present impact of all resources and technologies in planning period y [£M or $MtCO_2$]
$\mathscr{I}^{CO2price}_{iy}$	Total net present impact of the CO_2 price in planning period y [£M]
$\mathscr{I}^{\mathrm{P}}_{iy}$	Total net present impact of building new conversion technologies in planning period y [£M or $MtCO_2$]
$\mathscr{I}^{\mathrm{S}}_{iy}$	Total net present impact of building new storage technologies in planning period y [£M or $MtCO_2$]
$\mathscr{I}^{\mathrm{Q}}_{iy}$	Total net present impact of building new transport infrastructures in planning period y [£M or $MtCO_2$]
$\mathscr{I}^{\mathrm{L}}_{iy}$	Total net present impact of building new linepack connections in planning period y [£M or $MtCO_2$]
$\mathscr{I}^{\mathrm{W}}_{iy}$	Total net present capital impact of building new wind turbines in planning period y [£M or $MtCO_2$]
$\mathscr{I}^{\mathrm{SL}}_{iy}$	Total net present capital impact of building new solar PV installations in planning period y [£M or $MtCO_2$]
$\mathscr{I}^{\mathrm{m}}_{iy}$	Total net present impact of importing resources in planning period y [£M or $MtCO_2$]

$\mathscr{I}_{iy}^{\mathrm{fp}}$ Total net present fixed O&M impact of conversion technologies in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{fq}}$ Total net present fixed O&M impact of transport infrastructures in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{fs}}$ Total net present fixed O&M impact of storage technologies in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{fl}}$ Total net present fixed O&M impact of linepack connections in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{w}}$ Total net present O&M impact of wind turbines in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{sl}}$ Total net present O&M impact of solar PV installations in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{Rev}}$ Total net present revenue from the sales of energy services for satisfying demands in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{U}}$ Total impact of utilising natural resources in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{C}}$ Total impact of resource curtailment in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{vp}}$ Total net present variable operating impact of production facilities in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{vs}}$ Total net present variable operating impact of storage facilities in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{vq}}$ Total net present variable operating impact of transport technologies in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{vl}}$ Total net present variable operating impact of linepack connections in planning period y [£M or $\mathrm{MtCO_2}$]

$\mathscr{I}_{iy}^{\mathrm{x}}$ Total net present impact of exporting resources in planning period y [£M or $\mathrm{MtCO_2}$]

J_{lhdty} Inventory in linepack system l during hour h of day type d in season t of planning period y [UoR]

$J_{ldty}^{0,\mathrm{act}}$ Inventory in linepack system l at the start of day type d of season t in planning period y [UoR]

$J_{ldty}^{0,\mathrm{sim}}$ Inventory in linepack system l at the start of the simulated cycle for day type d of season t in planning period y [UoR]

M_{rzhdty} — Import rate of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]

N^{PD}_{pzy} — Millions of domestic conversion technology $p \in \mathbb{P}^{\mathrm{D}}$ in zone z in planning period y

U_{rzhdty} — Utilisation of natural resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]

$u^{\max}_{rzhdty}$ — Maximum availability of natural resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]

X_{rzhdty} — Export rate of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]

$\mathscr{P}^{\mathrm{h}}_{pzhdty}$ — Total rate of operation of hourly variable conversion technology p in zone z during hour h of day type d in season t of planning period y [MW]

$\mathscr{P}^{\mathrm{d}}_{pzdty}$ — Total rate of operation of daily variable conversion technology p in zone z during day type d in season t of planning period y [MW]

$\mathscr{Q}_{mzz'hdty}$ — Operation rate of transport technology l from zone z to zone z' during hour h of day type d in season t of planning period y [UoR/h]

$\mathscr{S}^{\mathrm{get}}_{szhdty}$ — Operation rate of “get” task by storage s in zone z during hour h of day type d in season t of planning period y [UoR/h]

$\mathscr{S}^{\mathrm{hold}}_{szhdty}$ — Operation rate of “hold” task by storage s in zone z during hour h of day type d in season t of planning period y [UoR/h]

$\mathscr{S}^{\mathrm{put}}_{szhdty}$ — Operation rate of “put” task by storage s in zone z during hour h of day type d in season t of planning period y [UoR/h]

$\mathscr{L}^{\mathrm{get}}_{lzhdty}$ — Operation rate of “get” task by linepack system l in zone z during hour h of day type d in season t of planning period y [UoR/h]

$\mathscr{L}^{\mathrm{hold}}_{lhdty}$ — Operation rate of “hold” task by linepack system l in zone z during hour h of day type d in season t of planning period y [UoR/h]

$\mathscr{L}^{\mathrm{put}}_{lzhdty}$ — Operation rate of “put” task by linepack system l in zone z during hour h of day type d in season t of planning period y [UoR/h]

Free variables

L_{zrhdty} — Net rate of transfer of resource r into zone z from the linepack transmission system during hour h of day type d in season t of planning period y [UoR/h]

P^{h}_{rzhdty}	Net rate of production by hourly variable technologies of resource r in zone z during hour h of day type d in season t of planning period y [UoR/h]
P^{d}_{rzdty}	Net rate of production by daily variable technologies of resource r in zone z during day type d in season t of planning period y [UoR/h]
P^{P,CO_2}_{y}	Total (net) production of CO_2 by conversion technologies in planning period y
Q_{rzhdty}	Net transport rate of resource r into zone z from all other zones during hour h of day type d in season t of planning period y [UoR/h]
S_{rzhdty}	Net production of resource r in zone z due to the operation of storage technologies during hour h of day type d in season t of planning period y [UoR/h]
Z	Objective function
$\delta^{\mathrm{d}}_{szdty}$	Net surplus put into storage s in zone z over one day in day type d in season t of planning period y [UoR]
$\delta^{\mathrm{t}}_{szty}$	Net surplus put into storage s in zone z over one week in season t of planning period y [UoR]
$\delta^{\mathrm{y}}_{szy}$	Net surplus put into storage s in zone z over one year in planning period y [UoR]
$\Delta^{\mathrm{d}}_{ldty}$	Net surplus put into linepack system l over one day in day type d in season t of planning period y [UoR]
$\Delta^{\mathrm{t}}_{lty}$	Net surplus put into linepack system l over one week in season t of planning period y [UoR]
Δ^{y}_{ly}	Net surplus put into linepack system l over one year in planning period y [UoR]

Integer variables

$N^{\mathrm{B}}_{bzz'y}$	Number of transport infrastructure b installed between zones z and z' during planning period y
N^{PC}_{pzy}	Total number of commercial conversion technology $p \in \mathbb{P}^{\mathrm{C}}$ in zone z during planning period y
N^{S}_{szy}	Total number of storage technology s in zone z during planning period y
N^{L}_{lzy}	Total number of connections of linepack system l in zone z during planning period y
N^{W}_{wzy}	Total number of wind turbines of type w in zone z during planning period y

N^{Sl}_{slzy}	Total number of solar PV installations of type sl in zone z during planning period y
$NI^{\mathrm{B}}_{bzz'y}$	Number of new transport infrastructure b invested in at the beginning of planning period y between zones z and z'
NI^{PC}_{pzy}	Number of new commercial conversion technology $p \in \mathbb{P}^{\mathrm{C}}$ invested in at the beginning of planning period y in zone z
NI^{S}_{szy}	Number of new storage facility s invested in at the beginning of planning period y in zone z
NI^{L}_{lzy}	Number of new connections of linepack system l invested in at the beginning of planning period y in zone z
NI^{W}_{wzy}	Number of new wind turbines of type w invested in at the beginning of planning period y in zone z
NI^{Sl}_{slzy}	Number of new solar PV installations of type sl invested in at the beginning of planning period y in zone z
NR^{PC}_{pzy}	Number of commercial conversion technology $p \in \mathbb{P}^{\mathrm{C}}$ retired in zone z at the beginning of planning period y
NR^{S}_{szy}	Number of storage facility s retired in zone z at the beginning of planning period y
NR^{L}_{lzy}	Number of connections of linepack system l retired in zone z at the beginning of planning period y
NR^{W}_{wzy}	Number of wind turbines of type w retired in zone z at the beginning of planning period y
NR^{Sl}_{slzy}	Number of solar PV installations of type sl retired in zone z at the beginning of planning period y

Appendix B

Value Web Model input data

This appendix has been included to provide information on the model input data that was used in the modelling described in this thesis. The majority of this appendix has been adapted from a data article that has been published by Elsevier in Data in Brief. The publisher permits the re-use of the article in this thesis, provided that the journal is referenced as the original source. The article details are as follows:

> Christopher J. Quarton and Sheila Samsatli. Resource and technology data for spatio-temporal value chain modelling of the Great Britain energy system *Data in Brief*, 31:105886. https://doi.org/10.1016/j.dib.2020.105886

Sections B.1 and B.2 have been adapted and re-formatted from the above article for this thesis, but the data remains the same as in the original article. The data in those sections was compiled for the study in Chapter 5. The same dataset was used for Chaper 6, with some minor changes; these changes are detailed in Section B.3 of this appendix. Each chapter has unique scenario designs and assumptions, so it is recommended to refer to the chapters, or original articles, for more detailed information.

B.1 Data

This appendix includes all of the input data used for a value chain optimisation of the GB energy system, including data for all of the energy resources and technologies that were modelled. Example resource data includes availability of primary resources (e.g. wind), and final energy demands (for electricity and heating). Technologies include those for the conversion of resources (e.g. electrolysers and turbines), transportation technologies (e.g. pipelines), and storage technologies (e.g. pressure vessels).

The value chain optimisation was carried out using the Value Web Model (VWM). The VWM is able to model a wide range of energy value chains by including data for a variety of resources and technologies. An optimisation can then be performed to find an optimal energy system design and operating strategy for satisfying final energy demands using the primary resources that are available.

The VWM has a spatial-temporal representation of the GB energy system, included 16 spatial zones and time intervals representing seasonal and sub-day variations, as well as long term (e.g. decadal) energy system evolution. The data presented in this article, in particular the resource data, is presented in the spatio-temporal aggregation of the VWM. Further details of the spatio-temporal format, as well as details of the processing carried out to convert data to this format, is provided in section B.2.

The remainder of this section provides the actual energy system data. Resource data, including availabilities and demands, is provided in subsection B.1.1. Technology data, including economic and operational parameters, is provided in subsection B.1.2.

B.1.1 Resource data

In this sub-section, data relating to the resources included in the VWM are presented. Resources represented in the VWM include:

- Primary resources that can be utilised by technologies in the model (e.g. wind and solar);
- The various resources associated with the operation of technologies (i.e. technology inputs and outputs);
- Resources that have final demands associated with them (e.g. electricity and heat).

B.1.1.1 Resource availability

Wind resource

The wind energy resource is represented with separate wind speed profiles for each spatial zone. Wind speed data was acquired from the Renewables Ninja database [4, 5], which specifies hourly

Table B.1: Hourly onshore wind speed profiles for each spatial zone in each season (m/s). Calculated from [4, 5]

s	h	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Spring	1	6.22	8.42	7.12	9.06	8.70	8.02	8.65	5.77	6.07	5.55	7.03	6.42	6.15	7.07	5.90	7.68
	2	7.56	8.00	8.55	8.19	8.72	8.98	7.95	5.88	6.16	5.35	8.70	6.45	5.71	7.62	5.98	5.28
	3	9.33	7.49	8.67	5.74	6.38	6.85	6.69	8.07	7.64	7.71	6.98	7.27	6.93	6.20	7.46	4.85
	4	8.26	6.72	6.14	5.99	5.74	5.59	4.60	7.50	6.85	6.86	4.99	6.33	7.01	6.31	7.17	8.71
Summer	1	7.93	6.63	7.75	5.07	4.80	5.13	6.17	6.92	8.21	5.42	4.93	6.35	7.06	6.37	6.31	5.78
	2	6.07	4.97	3.60	3.85	5.73	4.77	3.55	4.98	3.10	3.70	5.41	5.99	4.74	7.47	6.02	6.93
	3	4.50	3.22	3.03	5.90	6.34	5.50	4.65	5.07	2.98	4.64	6.08	5.80	4.35	6.78	6.55	6.94
	4	5.21	7.88	7.97	6.88	6.36	6.97	7.28	5.54	6.56	7.56	6.93	5.20	6.11	4.27	4.95	5.87
Autumn	1	8.77	7.38	7.81	6.66	7.62	7.63	7.51	6.98	5.97	8.15	7.28	8.77	8.43	6.67	5.99	6.50
	2	5.99	8.62	6.45	6.65	5.35	6.45	7.19	6.20	7.08	6.09	7.08	7.38	7.33	7.08	6.83	4.53
	3	4.86	7.90	6.10	7.08	5.81	6.21	6.80	5.98	8.08	4.30	6.96	5.61	5.12	7.82	7.75	6.24
	4	9.01	6.66	8.18	6.53	7.73	6.99	5.89	8.01	6.14	6.37	5.69	5.45	5.76	6.86	7.38	10.99
Winter	1	10.43	12.02	10.74	8.20	8.02	8.54	11.77	10.74	10.18	10.33	8.47	11.56	9.94	11.76	12.09	8.88
	2	11.62	12.76	11.78	7.59	9.55	9.60	9.87	10.03	9.88	7.65	9.56	11.52	11.84	8.84	9.95	9.61
	3	10.62	9.88	11.08	9.20	10.43	10.47	7.35	9.98	10.42	8.62	10.56	8.84	10.66	9.64	9.62	12.08
	4	8.85	7.35	7.30	11.06	10.94	10.98	9.90	9.10	8.94	9.72	11.46	8.32	8.65	10.73	8.94	12.28
Peak	1	8.92	7.69	8.12	7.20	6.21	7.37	8.18	8.25	9.03	7.83	8.85	8.11	7.27	8.45	7.49	9.97
	2	8.64	9.30	8.31	6.76	7.79	8.82	8.59	8.64	9.39	8.76	8.87	6.80	5.80	8.20	6.21	8.48
	3	7.34	9.82	7.97	6.72	8.59	7.39	7.45	7.44	7.07	7.84	7.61	7.29	6.99	8.36	7.59	7.02
	4	8.48	7.50	6.87	7.88	7.73	8.55	6.93	7.20	6.67	6.23	6.41	7.84	8.19	6.82	8.57	9.13

wind speeds for all locations in the UK in 2014. This data was processed to match the model spatial and temporal representation – details of this processing are provided in section 2.2.

In Table B.1 and Table B.2, the wind speed data is presented, for onshore and onshore installations respectively, in 2020. Wind speeds were assumed to grow by 2% per decade in Scotland (zones 1 to 5), and fall by 2% per decade in England and Wales (zones 6 to 16), based on Met Office data [6]. This is applied as a multiplication factor for each decade, compared to the first decade.

Solar resource

The solar resource is represented in a similar manner to the wind resource. The solar resource in the VWM is taken directly from the Renewables Ninja database [4], and represents the fraction of the panel's nominal capacity (i.e. in kW per kW capacity) that is expected at the given time and location. Further information about this data, including the temporal aggregation that was carried out, is provided in section B.2.3. The final irradiance profiles are shown in Table B.3. Long term changes in the solar resource were taken from the medium emissions scenario with 50% probability data calculated by Burnett et al. [7]. This data for each spatial zone is shown

Table B.2: Hourly offshore wind speed profiles for each spatial zone in each season (m/s). Calculated from [4, 5]

s	h	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Spring	1	8.88	10.47	11.31	9.41	10.24	11.63	8.68	8.86	12.38	-	11.10	8.46	-	7.98	8.87	7.65
	2	10.04	9.45	8.77	8.11	10.18	6.89	9.16	8.18	8.27	-	8.71	7.84	-	7.21	7.63	7.55
	3	11.35	9.65	8.86	8.07	9.63	6.78	9.83	8.67	7.02	-	7.21	8.63	-	8.26	8.21	9.01
	4	11.58	9.80	9.40	11.60	7.63	11.11	10.72	10.08	8.81	-	9.89	9.32	-	9.45	8.89	10.70
Summer	1	8.08	7.55	8.65	5.97	9.66	9.05	9.63	8.38	7.37	-	7.75	7.58	-	6.77	9.60	9.09
	2	8.35	6.72	8.16	8.05	9.84	8.98	9.87	9.55	8.95	-	6.76	9.04	-	7.18	8.70	7.47
	3	9.97	8.50	10.03	8.68	7.77	7.58	8.95	8.66	8.23	-	9.11	9.03	-	8.39	6.21	7.81
	4	8.58	9.92	7.83	8.51	6.98	6.33	6.15	7.07	9.40	-	9.61	7.28	-	9.06	7.07	7.66
Autumn	1	9.87	9.32	12.58	8.86	8.27	9.10	8.80	9.71	10.17	-	9.56	11.21	-	9.16	9.99	8.78
	2	9.64	7.67	10.23	7.07	7.44	9.06	8.80	11.89	7.36	-	7.89	9.51	-	9.80	10.94	7.19
	3	10.90	10.27	8.62	7.95	10.81	9.25	9.33	10.08	9.98	-	6.62	7.32	-	7.87	9.09	9.86
	4	12.02	12.65	7.57	11.84	10.58	10.23	10.74	8.06	8.76	-	12.62	9.14	-	8.77	6.82	11.33
Winter	1	11.61	11.93	12.76	12.59	10.72	10.76	12.99	11.62	13.28	-	13.26	14.41	-	13.55	10.73	15.63
	2	12.29	14.75	13.77	14.98	12.92	11.86	11.48	14.90	14.54	-	14.94	11.87	-	12.68	11.13	14.89
	3	15.01	14.51	13.56	12.36	13.58	13.27	12.01	13.95	14.04	-	14.41	11.10	-	11.78	12.86	13.48
	4	14.72	11.70	12.10	9.71	12.74	13.69	14.10	13.33	10.44	-	11.83	12.08	-	11.05	13.85	9.59
Peak	1	10.17	10.69	9.39	10.09	11.28	11.72	11.13	11.46	12.83	-	11.57	9.10	-	9.94	8.49	11.53
	2	10.77	12.84	10.52	8.00	10.54	11.08	8.65	11.39	9.85	-	7.54	10.40	-	9.66	8.00	10.36
	3	11.90	11.16	11.78	10.26	9.26	9.54	10.49	10.28	9.53	-	11.34	11.10	-	8.83	8.95	8.50
	4	12.08	8.96	9.94	10.30	8.40	8.68	11.33	9.53	10.64	-	10.80	10.07	-	10.08	11.78	12.23

in Table B.4 for 2050; intervening years can be linearly interpolated.

Natural gas resource

Availability of natural gas is included, from both UK-based production and imports via interconnector pipelines and liquefied natural gas (LNG). The maximum utilisation rates of natural gas from production or import in each spatial zone are assumed constant throughout the year, and are shown in Table B.5.

Production of natural gas is from the North Sea: the maximum utilisation potential is based on National Grid data [8]. Pipeline and LNG import capacities are estimated from the capacity of existing facilities, including from Norway (3 pipelines), continental Europe (2 pipelines), and as LNG (terminals at Milford Haven and the Isle of Grain) [9]. Capacities are converted from cubic metres based on a higher heating value of 10.97 kWh/m^3.

A steady cost for gas import or production of £17.6 /MWh is assumed based on the average UK day-ahead wholesale price for 2018 [10]. The GHG (CO2 -equivalent) emissions associated with

Table B.3: Hourly solar irradiance profiles for each spatial zone in each season (expressed as a fraction of the panel nominal capacity). Calculated from [4].

s	h	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Spring	1	0.002	0.002	0.002	0.001	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.001	0.002	0.002	0.002	0.001
	2	0.132	0.150	0.140	0.124	0.133	0.154	0.176	0.172	0.183	0.165	0.205	0.158	0.204	0.243	0.199	0.167
	3	0.426	0.433	0.433	0.403	0.414	0.440	0.487	0.520	0.504	0.496	0.534	0.496	0.547	0.611	0.558	0.507
	4	0.084	0.086	0.092	0.085	0.083	0.076	0.079	0.095	0.080	0.086	0.083	0.087	0.089	0.094	0.092	0.100
Summer	1	0.006	0.007	0.005	0.006	0.006	0.007	0.007	0.006	0.007	0.006	0.006	0.005	0.006	0.007	0.006	0.004
	2	0.210	0.243	0.229	0.237	0.242	0.263	0.278	0.265	0.279	0.274	0.280	0.257	0.285	0.306	0.286	0.253
	3	0.490	0.520	0.555	0.529	0.532	0.552	0.561	0.617	0.562	0.578	0.568	0.591	0.584	0.621	0.604	0.602
	4	0.124	0.117	0.143	0.123	0.124	0.123	0.120	0.147	0.116	0.124	0.113	0.133	0.115	0.122	0.121	0.142
Autumn	1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2	0.040	0.056	0.053	0.050	0.053	0.067	0.081	0.075	0.086	0.077	0.093	0.073	0.093	0.110	0.091	0.074
	3	0.259	0.278	0.307	0.279	0.299	0.325	0.360	0.383	0.358	0.354	0.368	0.351	0.379	0.412	0.384	0.373
	4	0.033	0.033	0.042	0.034	0.038	0.039	0.038	0.047	0.037	0.039	0.036	0.044	0.041	0.043	0.045	0.049
Winter	1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2	0.004	0.005	0.003	0.003	0.003	0.006	0.009	0.009	0.010	0.008	0.010	0.009	0.010	0.018	0.015	0.012
	3	0.092	0.112	0.099	0.081	0.095	0.125	0.168	0.171	0.188	0.180	0.199	0.193	0.215	0.238	0.235	0.210
	4	0.004	0.004	0.005	0.004	0.004	0.005	0.007	0.008	0.007	0.009	0.008	0.010	0.010	0.010	0.012	0.012
Peak	1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2	0.004	0.005	0.003	0.003	0.003	0.006	0.009	0.009	0.010	0.008	0.010	0.009	0.010	0.018	0.015	0.012
	3	0.092	0.112	0.099	0.081	0.095	0.125	0.168	0.171	0.188	0.180	0.199	0.193	0.215	0.238	0.235	0.210
	4	0.004	0.004	0.005	0.004	0.004	0.005	0.007	0.008	0.007	0.009	0.008	0.010	0.010	0.010	0.012	0.012

Table B.4: Factors to apply to solar resource to represent long term climate change. Data from [7].

	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Factor (2050)	1.00	1.00	1.01	1.01	1.02	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.05	1.05	1.05	1.05

Table B.5: Availability of natural gas from UK-based production and imports via pipeline and LNG [8, 9].

	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Production capacity (MW)	0	48,500	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Import capacity (MW)	0	36,700	0	0	0	0	32,900	0	0	0	50,700	36,400	0	25,000	0	0

Table B.6: Available land, seabed and rooftop area for wind turbines (onshore and offshore) and solar PV installations (farms and rooftops) [12, 3, 13, 14].

Available area (km^2)	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Onshore wind turbines	74	141	7	147	420	260	356	601	168	281	446	617	61	71	159	444
Offshore wind turbines	2140	182	418	572	545	2330	1670	1590	1010	0	1110	903	0	621	793	1610
Solar farms	2376	929	107	3254	3714	4803	835	6240	6343	3574	322	2918	2243	3103	167	938
Rooftop solar	4.8	4.8	0.7	10.1	19.1	20.0	36.4	50.4	10.5	42.1	37.4	44.3	42.1	14.2	26.3	26.2

the production of natural gas (whether from UK production or imports) are also included, with a value of 0.013 tCO_2 /MWh [11].

Land availability

Wind turbines and solar PV can only be installed in the model if there is enough available land, seabed and rooftop areas. The available areas are shown in Table B.6.

The available land and seabed area for new wind turbines was based on land suitability analyses performed by Samsatli and co-workers (onshore [12]; offshore [3]).

The available land area for new solar farms was taken from a land suitability analysis performed at part of an MSc thesis by Martinez Diaz at the University of Bath.

The available area for rooftop solar was estimated from the total area of buildings in the UK, by processing Ordnance Survey Open Map data [13]. These per-zone areas were divided by a factor of 8, to account for rooftops that are not suitable for solar PV or have an unsuitable orientation. This approach is similar to that used by Mackay [14].

B.1.1.2 Resource demands

Electricity

Electricity demands from the domestic, commercial and industrial sectors are included. Annual levels of demand in each of these sectors in 2020, as well as the spatial distribution of these demands, was taken from data from the UK Department for Business Energy and Industrial Strategy (BEIS) [15, 16]. The spatial distribution was aggregated into the 16 modelled spatial zones, and the resulting totals for each zone are shown in Figure B-1.

The time profiles for electricity demand in each sector were estimated from Sustainability First [17], and aggregated into the model time resolution by averaging. These aggregated electricity demands are shown in Table B.7. When demands for electricity are satisfied, a revenue to the overall energy system is accounted, based on an electricity price of £46/MWh [18]. Future projections for electricity demand were made based on the National Grid Future Energy Scenarios [19], using the Steady Progression scenario for domestic and commercial demands, and the 2 degrees scenario for industrial demands. In these scenarios, domestic demand grows by 28% by 2050; commercial demand grows by 5%; and industrial demand grows by 6% (therefore overall electricity demand grows by 13%).

Heat

Heat demands are represented in a similar manner to electricity demands, except that demands are separated into three groups, so that the different technologies used to generate heat in each sector can be modelled separately. All heat demand data, including annual totals for each sector, spatial spread, and hourly demand profiles were taken from data provided by the BEIS Heat Strategic Options project [20]. This data is protected by a non-disclosure agreement so cannot be reproduced here. As an indication, the three sector groupings are shown below, with the total annual heat demands from each sector:

- Domestic heat (339.1 TWh/year);
- Commercial and low-temperature industrial heat (233.0 TWh/year);
- High-temperature industrial heat (117.8 TWh/year).

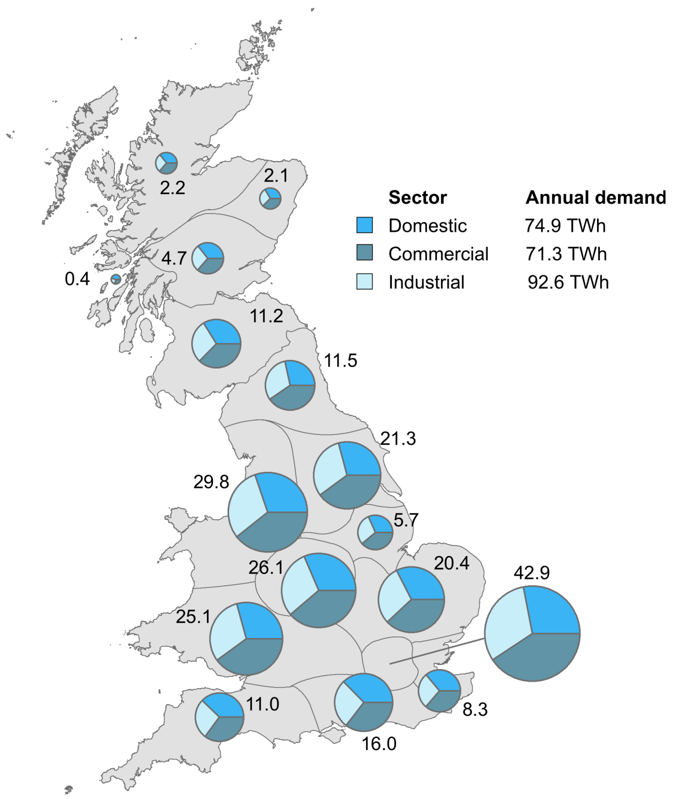


Figure B-1: Map showing baseline (2020) annual demands for electricity in each spatial zone, differentiated by sector. Calculated from [15, 16].

Table B.7: Aggregated electricity demands (all sectors) (MW). Calculated from [15, 16, 17].

s	h	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Spring	1	197	186	38	422	1008	1030	1907	2670	512	2336	1835	2246	3829	750	1442	995
	2	245	232	47	527	1261	1295	2396	3352	642	2929	2299	2822	4817	937	1798	1239
	3	267	254	50	574	1379	1434	2649	3697	706	3223	2522	3120	5343	1019	1951	1343
	4	270	255	53	581	1386	1413	2618	3667	704	3210	2522	3083	5254	1032	1986	1370
Summer	1	170	162	32	365	876	909	1680	2345	448	2045	1601	1978	3386	648	1241	854
	2	214	203	40	459	1103	1145	2116	2954	564	2575	2016	2492	4266	815	1561	1075
	3	248	237	46	533	1285	1343	2480	3457	659	3010	2352	2920	5008	947	1811	1246
	4	245	233	47	527	1262	1299	2403	3360	643	2935	2301	2830	4834	936	1796	1238
Autumn	1	196	186	37	421	1009	1038	1921	2685	514	2346	1840	2262	3864	748	1436	990
	2	247	235	47	530	1272	1313	2429	3394	649	2962	2322	2860	4890	943	1807	1245
	3	275	262	51	590	1421	1483	2737	3817	729	3324	2600	3223	5525	1048	2004	1380
	4	285	269	55	612	1460	1488	2756	3861	741	3381	2657	3246	5532	1088	2092	1443
Winter	1	236	223	46	508	1210	1229	2279	3194	613	2798	2200	2684	4570	903	1737	1199
	2	282	267	54	605	1447	1485	2748	3844	737	3360	2637	3236	5524	1075	2064	1423
	3	309	294	58	663	1592	1650	3049	4257	814	3714	2908	3591	6145	1178	2256	1554
	4	325	306	64	698	1662	1680	3116	4372	841	3834	3018	3670	6241	1242	2393	1652
Peak	1	253	239	49	543	1298	1328	2458	3442	660	3010	2364	2895	4938	966	1855	1279
	2	298	282	56	639	1532	1581	2923	4085	782	3567	2796	3442	5884	1136	2178	1501
	3	330	315	62	710	1707	1777	3282	4578	874	3990	3121	3865	6620	1261	2412	1661
	4	345	325	67	740	1764	1789	3317	4651	894	4076	3206	3907	6651	1316	2534	1748

When demands for heat are satisfied, a revenue to the overall energy system is accounted, based on a heat price of £34/MWh [21].

B.1.2 Technology data

In this subsection, data for the technologies included in the VWM are presented. Data for a wide range of technologies are included, including technologies for:

- Utilising primary resources (e.g. wind turbines generating electricity from the wind);
- Converting between resources (e.g. electrolysers converting from electricity to hydrogen);
- Transporting resources between spatial zones;
- Storing resources.

Table B.8: Wind turbine data [22, 23, 24, 25, 26]

Parameter		Onshore	Existing offshore	New offshore
Radius (m)		45	63	110
Rated power (MW)		2.3	5.1	12.0
Rated wind speed (m/s)		13.0	14.0	13.0
Cut-in wind speed (m/s)		3.0	3.5	3.5
Cut-out wind speed (m/s)		25.0	30.0	30.0
Unit CAPEX (£M_{2017})		3.0	-	29.0
Unit fixed OPEX (£M_{2017} /yr)		0.22	-	1.15
Unit variable OPEX (£M_{2017} /MWh)		0	0	0
Cost learning factor	2030	0.94	-	0.91
	2040	0.90		0.88
	2050	0.90		0.86
Lifetime (yrs)		20	20	20

B.1.2.1 Resource utilisation technologies

Resource utilisation technologies are those that convert the primary resources described in Section B.1.1.1 into resources usable in the energy system, and include wind turbines and solar PV installations.

Wind turbine data

Wind turbines are represented with "typical" wind turbine types. For onshore turbines, a single turbine type is included, for which data is based on the Nordex N90 (2.3 MW) turbine [22]. For offshore wind turbines, two turbine types are included: one for existing offshore wind turbines and one for new offshore turbines, in order to represent the larger turbine sizes expected in the future. The existing offshore turbine data is based on the REpower 5M (5.075 MW) turbine [23], whilst for new offshore wind turbines the data based on the General Electric Haliade-X turbine (12.0 MW) [24], except for power curve information which was estimated. For all turbines, current cost data was based on BEIS data [25]. The future cost reduction factor is a multiplier to be applied to present day costs to represent future costs, and was estimated from [26]. "Lifetime" represents both the technical lifetime over which the turbine operates, and the economic lifetime over which the initial capital expenditure is paid off. All data for these turbines are shown in Table B.8.

Table B.9: Solar PV panel installation data [25, 27, 28, 29, 30]

Parameter		Farm PV	Rooftop PV
Panel unit size (MW)		1	1
Unit land footprint (km^2)		0.02	0.007
Siting factor		1	0.8
System efficiency		85%	85%
Unit CAPEX (£M_{2017})		0.67	0.72
Unit fixed OPEX (£M_{2017} /yr)		0.0067	0.0076
Unit variable OPEX (£$_{2017}$ /MWh)		0	0
Cost learning factor	2030	0.85	0.85
	2040	0.75	0.75
	2050	0.67	0.67
Lifetime (yrs)		20	20

Solar PV data

For solar PV, separate technology data are included for solar PV farms and rooftop solar PV. These data are shown in Table B.9. A nominal installation size of 1 MW capacity is used (but multiple units can be installed at once, for larger installations). The land (or rooftop) footprint includes the panel itself and any additional space requirements for ancillary equipment, and is taken from [27] (PV farm) and [28] (rooftop, assuming a 40° roof tilt). The siting factor is an efficiency factor applied to panel power output based on the panel position: for PV farms, it is assumed that an optimal orientation is used (i.e. factor = 1), whilst for rooftop installations, siting is assumed to be 80% optimal. Overall system efficiencies were set to achieve realistic load factors based on BEIS solar data [29]. Current cost data was also taken from BEIS data [25], whilst future cost reductions were taken from [30].

Existing wind and solar installations

The installed capacities of existing wind and solar installations are modelled, including the capacity installed in 2020 and accounting for retirements in future decades. This data was compiled from the BEIS Renewable Energy Planning Database [31] and the BEIS Solar photovoltaics deployment database [32]; more details of how the data was compiled are provided in section B.2.4. The final data is shown in Table B.10.

Table B.10: Installed capacities of existing wind turbines and solar PV in 2020, and remaining capacity in 2030. All values in MW. Estimated from [31, 32].

Available area (km^2)		Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Onshore	2020	1859	1017	36	447	3938	1330	656	452	181	222	533	933	13	164	8	242
wind turbines	2030	1507	825	32	342	2952	979	576	315	91	150	382	704	7	104	8	212
Offshore	2020	598	123	0	7	0	108	1629	2904	1037	0	1493	0	0	2047	465	0
wind turbines	2030	588	123	0	7	0	104	1629	2490	843	0	1433	0	0	1849	400	0
Solar farms	2020	0	11	0	57	6	117	314	277	551	587	1465	1938	8	567	687	1611
	2030	0	11	0	57	6	117	314	277	551	587	1465	1938	8	567	687	1611
Rooftop solar	2020	0	1	0	11	2	43	209	256	106	452	1002	1568	6	147	331	771
	2030	0	1	0	11	2	43	209	256	106	452	1002	1568	6	147	331	771

B.1.2.2 Conversion technologies

Conversion technologies convert between different resources within the energy system: for example, an electrolyser converts electricity to hydrogen, whilst a gas turbine converts natural gas to electricity and CO_2. Technological and economic information for all of the technologies that are included are shown in Table B.11. For some technologies, different sizes are included. The conversion factors describe the consumption and production of resource when the technology is operating: for example, for an electrolyser, 1.667 MWh of electricity is consumed for each 1 MWh of hydrogen production. Operating flexibility describes whether the technology is able to vary its output on an hourly basis, or only a daily basis (due to the model temporal representation, "daily" effectively represents seasonal variation). Cost data is provided for 2020, and these costs can be multiplied by the cost learning factors to provide estimates of future costs. "Lifetime" represents both the technical lifetime over which the turbine operates, and the economic lifetime over which the initial capital expenditure is paid off. The references used for each technology are also included in Table B.11.

Existing installed capacities of some technologies are also included, and this data is shown in Table B.12. This data was compiled from various sources, including [15, 20, 33, 34, 35]. Details of how this data was compiled are provided in section B.2.5.

Table B.11: Technical and economic data for conversion technologies. References provided within the table.

Technology		Electrolyser (S)	Electrolyser (L)	SMR + CC (S)	SMR + CC (L)	NG CCGT	NG CCGT + CC	NG OCGT	NG OCGT + CC	H2 CCGT	H2 OCGT	H2 Fuel Cell (S)	H2 Fuel Cell (L)
	Electricity	− 1.667	− 1.667			+ 1.000	+ 1.000	+ 1.000	+ 1.000	+ 1.000	+ 1.000	+ 1.000	+ 1.000
	Hydrogen	+ 1.000	+ 1.000	+ 1.000	+ 1.000					− 1.667	− 2.564	− 2.000	− 1.754
	Nat. Gas			− 1.447	− 1.447	− 1.667	− 1.895	− 2.564	− 2.915				
	Elec (distributed)												
	Hydrogen (distributed)												
	Nat. Gas (distributed)												
Resource	Hydrogen (high pressure)												
conversions	Nat. Gas (high pressure)												
	Heat (industrial)												
	Heat (commercial)												
	Heat (domestic)												
	Captured CO2			+ 0.267	+ 0.267		+ 0.307		+ 0.473				
	Emitted CO2			+ 0.030	+ 0.030	+ 0.300	+ 0.034	+ 0.462	+ 0.053				
	Stored CO2												
Max operating rate (MW)		10	100	300	1000	1200	1036	625	539	1200	625	10	100
Min operating rate (MW)		0	0	210	700	0	0	0	0	0	0	0	0
Operating flexibility		Hourly	Hourly	Daily	Daily	Daily	Daily	Hourly	Hourly	Daily	Hourly	Hourly	Hourly
Capex (£M2017)		12.5	100	243	529	657	1290	225	441	723	248	4.66	46.6
Fixed opex (£M2017/yr)		0.375	3	9	30	15.3	30	3.01	5.9	16.8	3.31	0.233	2.33
Variable opex (£2017/MWh)		Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible
Lifetime (yrs)		15	15	25	25	25	25	25	25	25	25	10	10
Cost	2030	0.6	0.6	0.88	0.88	0.97	0.92	0.97	0.92	0.90	0.90	0.64	0.64
learning	2040	0.5	0.5	0.78	0.78	0.93	0.86	0.93	0.86	0.85	0.85	0.58	0.58
factor	2050	0.45	0.45	0.68	0.68	0.90	0.80	0.90	0.80	0.82	0.82	0.52	0.52
Ref.		[36, 37, 38]	[36, 37, 38]	[37, 39]	[37, 39]	[25]	[25]	[25, 40]	[25, 40]	[25]	[25]	[41]	[41]

Table B.11: *(Continued)*. Technical and economic data for conversion technologies. References provided within the table.

Technology		NG boiler (Ind)	H2 boiler (Ind)	Electric heater (Ind)	NG boiler (Com)	H2 boiler (Com)	Heat pump (Com)	Electric heater (Com)	NG boiler (Dom)	H2 boiler (Dom)	Heat pump (Dom)	Electric heater (Dom)
	Electricity			− 1.010								
	Hydrogen		− 1.090							− 1.090		
	Nat. Gas	− 1.090										
	Elec (distributed)						− 0.250	− 1.010			− 0.400	− 1.000
	Hydrogen (distributed)					− 1.090						
	Nat. Gas (distributed)				− 1.090				− 1.090			
Resource	Hydrogen (high pressure)											
conversions	Nat. Gas (high pressure)											
	Heat (industrial)	+ 1.000	+ 1.000	+ 1.000								
	Heat (commercial)				+ 1.000	+ 1.000	+ 1.000	+ 1.000				
	Heat (domestic)								+ 1.000	+ 1.000	+ 1.000	+ 1.000
	Captured CO2											
	Emitted CO2	+ 0.196			+ 0.196				+ 0.196			
	Stored CO2											
Max operating rate (MW)		50	50	10	10	10	10	10	0.028	0.028	0.028	0.028
Min operating rate (MW)		0	0	0	0	0	0	0	0	0	0	0
Operating flexibility		Hourly	Hourly	Hourly	Hourly	Hourly	Hourly	Hourly	Hourly	Hourly	Hourly	Hourly
Capex (£M2017)		9.84	11.8	1.22	1.69	2.03	3.06	1.22	0.00140	0.004	0.006	0.004
Fixed opex (£M2017/yr)		0.197	0.236	0.0245	0.0338	0.0405	0.0612	0.0245	0.00008	0.000096	0.00004	0.00004
Variable opex (£2017/MWh)		Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible
Lifetime (yrs)		25	20	15	25	20	20	20	20	20	20	20
Cost	2030	1.00	0.94	1.00	1.00	0.94	1.00	1.00	1.00	0.90	0.90	1.00
learning	2040	1.00	0.88	1.00	1.00	0.88	1.00	1.00	1.00	0.75	0.75	1.00
factor	2050	1.00	0.83	1.00	1.00	0.83	1.00	1.00	1.00	0.60	0.60	1.00
Ref.		[33]	[33]	[33]	[33]	[33]	[33]	[33]	[42]	[42, 43]	[43]	[43]

Table B.11: *(Continued)*. Technical and economic data for conversion technologies. References provided within the table.

Technology		NG CHP	NG CHP + CC	H2 CHP	Nuclear (S)	Nuclear (L)	CO2 Well (S)	CO2 Well (L)	H2 Compressor	H2 Expander	NG Compressor	NG Expander
	Electricity	+ 1.000	+ 1.000	+ 1.000	+ 1.000	+ 1.000			− 0.017	+ 0.009	− 0.017	+ 0.009
	Hydrogen			− 2.941					− 1.000	+ 1.000		
	Nat. Gas										− 1.000	+ 1.000
	Elec (distributed)											
	Hydrogen (distributed)											
	Nat. Gas (distributed)	− 2.941	− 3.401									
Resource	Hydrogen (high pressure)								+ 1.000	− 1.000		
conversions	Nat. Gas (high pressure)										+ 1.000	− 1.000
	Heat (industrial)											
	Heat (commercial)	+ 1.471	+ 1.471	+ 1.471								
	Heat (domestic)											
	Captured CO2		+ 0.535				− 1.000	− 1.000				
	Emitted CO2	+ 0.529	+ 0.066									
	Stored CO2						+ 1.000	+ 1.000				
Max operating rate (MW)		168	145	168	300	1600	228	571	100	100	330	330
Min operating rate (MW)		0	0	0	90	480	22.8	57.1	0	0	0	0
Operating flexibility		Hourly	Hourly	Hourly	Daily	Daily	Hourly	Hourly	Daily	Daily	Daily	Daily
Capex (£M2017)		139	237	153	1810	8130	137	231	0.7	1.1	0.7	1.1
Fixed opex (£M2017/yr)		4.67	7.96	5.14	13.4	60	6.49	7.67	0.035	0.055	0.035	0.055
Variable opex (£2017/MWh)		Negligible	Negligible	Negligible	5.00	5.00	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible
Lifetime (yrs)		25	25	25	40	40	40	40	20	20	20	20
Cost	2030	0.97	0.92	0.9	0.9	0.98	0.98	0.98	1.00	1.00	1.00	1.00
learning	2040	0.93	0.86	0.85	0.75	0.96	0.96	0.96	1.00	1.00	1.00	1.00
factor	2050	0.9	0.8	0.82	0.6	0.95	0.94	0.94	1.00	1.00	1.00	1.00
Ref.		[25]	[25, 40]	[25]	[44]	[45]	[46, 47]	[46, 47]	[21]	[21]	[21]	[21]

Table B.12: Installed capacities of existing conversion technologies in 2020, and remaining capacity in 2030. All values in MW. Estimated from various sources [15, 20, 33, 34, 35].

Installed capacity (MW)		Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
NG	2020	0	0	0	0	0	0	1,330	969	1,770	0	0	3,050	0	1,520	920	905
CCGT	2030	0	0	0	0	0	0	0	969	0	0	0	0	0	0	0	0
NG boiler	2020	97	146	16	421	955	1,830	335	1,130	1,760	152	222	991	1	34	176	1
(Ind)	2030	49	73	8	210	477	914	167	563	878	76	111	495	1	17	88	0
NG boiler	2020	250	1,040	50	2,640	5,530	4,160	5,100	16,200	8,440	5,610	4,350	1,900	7,240	3,310	3,680	3,760
(Com)	2030	125	520	25	1,320	2,770	2,080	2,550	8,120	4,220	2,810	2,180	950	3,620	1,660	1,840	1,880
NG boiler	2020	523	5,930	213	14,800	27,300	30,900	54,100	77,800	11,900	63,100	41,800	52,500	77,200	22,800	35,000	22,300
(Dom)	2030	262	2,960	106	7,380	13,700	15,500	27,100	38,900	5,960	31,500	20,900	26,300	38,600	11,400	17,500	11,200

B.1.2.3 Distribution technologies

Distribution technologies are those that convert general, centralised resources to the "distributed" resources that can be used by homes and businesses, such as gas and electricity distribution networks. These distribution technologies are represented in a similar manner to conversion technologies, although storage capacity can also be represented, for the linepack storage of gas distribution grids. The distribution technologies are represented in the model with a fixed size based on the maximum energy throughput, but multiple instances of the same technology can be installed within one spatial zone.

Electricity distribution grids represent the distribution networks that distribute centralised electricity (e.g. from power stations or the transmission system) to homes and businesses. Each electricity distribution technology installed in the model has a maximum capacity of 200 MW, but multiple technologies can be installed within one zone. Electricity losses were taken from [48]. Cost data was taken from [49].

Heat networks can deliver commercial grade heat, from combined heat and power and commercial heating plants, directly to buildings that are connected to the heating network. Cost and energy loss data is from [50], and accounts for the costs of connecting buildings to the heat network.

Natural gas distribution networks represent the local distribution systems that deliver gas from the national transmission system to homes and businesses. In addition to the delivery function of these networks, they also have an inherent linepack storage capacity, as the overall pressure level in the system can be varied, altering the total quantity of gas stored within the system. Natural gas distribution costs are from [51]. The linepack storage capacity for each section of natural gas grid was estimated by comparing the overall linepack capacity of the distribution system [52] with the makeup of the system to determine an approximate average storage level per MW of delivery capacity. Based on national gas statistics [15], gas distribution losses are assumed negligible compared to gas throughput.

Data for hydrogen distribution grids is based on the natural gas distribution data described above, with alterations based on the lower energy density of hydrogen compared to natural gas.

Finally, injection of hydrogen into existing natural gas distribution grids is also included, either through partial injection (mixing with natural gas), or complete conversion of the network to hydrogen.

For partial injection of hydrogen, the data shown in Table B.13 represents injection of hydrogen at a fixed rate of 7% by energy (equal to 20% by volume); the model formulation allows for variable operation of this injection, to allow for varying partial injection up to this 7% rate. The maximum throughput of the gas network with hydrogen injection is reduced (from 200 MW to 186 MW), due to the lower energy density and differing flow properties of hydrogen compared to natural gas. Modelling of storage for this technology is not required, as it is already modelled within the existing natural gas operation. Cost data is for the costs of any grid checks and upgrades that are required, and the injection equipment that controls the partial mixing of hydrogen into the natural gas. This data is taken from estimates made for the HyNet NW project [53].

For complete conversion of gas grids to hydrogen, the network throughput is also reduced. Cost data represents the costs of grid upgrades for converting to hydrogen; operational costs are already included in the existing gas grid infrastructure and are assumed to remain the same. The conversion costs are taken from the H21 project [54]. Existing natural gas and electricity distribution grids are also included; the data is shown in Table B.14. The existing capacity of electricity networks in each zone is based on the present-day peak electricity demand for that zone during the year (Table B.7). The existing capacity for natural gas distribution networks is estimated from the average gas offtake from the national gas transmission system at each local distribution zone (LDZ) exit point on the peak demand day (data from [8]). The average offtake for each exit point on its peak day was scaled by 1.6, to account for the peak hourly demand on that day. Due to the long lifetime of distribution infrastructures, no retirements of these technologies are modelled.

Table B.13: Technical and economic data for distribution technologies. References provided within the table.

Technology		Electricity distribution grid	Heat network	Natural gas distribution grid	H2 distribution grid	Partial H2 injection into gas grid	Conversion of gas grid to H2
	Electricity	− 1.060					
	Hydrogen				− 1.000	− 0.070	− 1.000
	Nat. Gas			− 1.000		− 0.930	
Resource	Elec (distributed)	+ 1.000	− 0.030				
conversions	Hydrogen (distributed)				+ 1.000		+ 1.000
	Nat. Gas (distributed)			+ 1.000		+ 1.000	
	Heat (commercial)		− 1.110				
	Heat (domestic)		+ 1.000				
Max operating rate (MW)		200	1	200	200	186	142
Min operating rate (MW)		0	0	0	0	0	0
Max energy storage capacity (MWh)		0	0	616	160	-	-
Min energy storage capacity (MWh)		0	0	439	114	-	-
Operating flexibility		Hourly	Hourly	Hourly	Hourly	Hourly	Hourly
Capex (£M2017)		130	1.08	267	267	0.72	0.68
Fixed opex (£M2017/yr)		3.9	0.0324	8.0	8.0	0.0216	0
Variable opex (£2017/MWh)		Negligible	Negligible	Negligible	Negligible	Negligible	Negligible
Lifetime (yrs)		40	40	40	40	40	40
Cost	2030	1.00	1.00	1.00	1.00	1.00	1.00
learning	2040	1.00	1.00	1.00	1.00	1.00	1.00
factor	2050	1.00	1.00	1.00	1.00	1.00	1.00
Ref.		[48, 49]	[50]	[51, 52]	[51, 52]	[51, 52, 53]	[51, 52, 54]

Table B.14: Existing natural gas and electricity distribution capacity. All values in MW. Estimated from [8] and Table B.7.

Installed capacity (MW)	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Natural gas distribution	334	5950	0	312	13300	12600	26200	33000	10400	27300	20500	33300	48100	4670	8560	6440
Electricity distribution	396	374	78	852	2030	2060	3820	5360	1030	4690	3690	4500	7660	1510	2910	2010

Table B.15: Hydrogen and natural gas storage technology data [37, 54, 56].

Technology		Underground H2 Storage (S)	Underground H2 Storage (L)	Low Pressure H2 Pressure Vessel	High Pressure H2 Pressure Vessel	Underground NG Storage (S)	Underground NG Storage (L)	Low Pressure NG Pressure Vessel	High Pressure NG Pressure Vessel
Max injection rate (MW)		400	1200	100	100	1320	3960	330	330
Min withdrawal rate (MW)		400	1200	100	100	1320	3960	330	330
Max storage capacity (MWh)		288,000	1,010,000	325	325	950,000	3,330,000	325	325
Min storage capacity (MWh)		86,400	303,000	0	0	285,000	1,000,000	0	0
Operating flexibility		Daily	Daily	Hourly	Hourly	Daily	Daily	Hourly	Hourly
Capex (£M2017)		104	248	3.72	17.8	104	248	3.72	17.8
Fixed opex (£M2017/yr)		3.8	9.2	0.111	0.345	3.8	9.2	0.111	0.345
Variable opex (£2017/MWh)		Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible	Negligible
Lifetime (yrs)		40	40	40	40	40	40	40	40
Cost learning factor	2030	1.00	1.00	1.00	0.90	1.00	1.00	1.00	0.90
	2040	1.00	1.00	0.95	0.75	1.00	1.00	0.95	0.75
	2050	1.00	1.00	0.90	0.65	1.00	1.00	0.90	0.65
Spatial zones		6, 7, 8, 9, 10, 15, 16	6, 7, 8, 9, 10, 15, 16	All	All	6, 7, 8, 9, 10, 15, 16	6, 7, 8, 9, 10, 15, 16	All	All

B.1.2.4 Storage technologies

Data for technologies for storing hydrogen and natural gas are included, and are shown in Table B.15.

Hydrogen storage options include high pressure underground storage (e.g. in salt caverns or depleted gas fields), and pressurised vessel storage. Technical and economic data for underground storage is based on H21 North of England data [54], which is in line with other references [37, 55]. Underground storage is only available in zones that have suitable geology [56]. Two above ground pressurised vessel storage technologies are also included: a low pressure storage and a high pressure storage; data for these technologies are from [37].

These storage options also exist for natural gas, and the data assumptions are the same, except that the higher energy density of natural gas enables larger quantities of energy to be stored in the same storage vessel.

Table B.16: Transport technology data [47, 53, 57, 58].

Technology		High Voltage AC Electricity Transmission, Single Circuit	High Voltage AC Electricity Transmission, Double Circuit	CO2 Pipeline
Max transport capacity (MW or t/hr)		750	1500	665
Losses per km (% / km)		0.013	0.013	0
Capex (£M2017)		400,000	750,000	2,030,000
Fixed opex (£M2017/yr)		7,000	13,000	60,900
Variable opex (£2017/MWh)		Negligible	Negligible	Negligible
Lifetime (yrs)		40	40	40
Cost	2030	1.00	1.00	1.00
learning	2040	1.00	1.00	1.00
factor	2050	1.00	1.00	1.00

B.1.2.5 Transportation technologies

Transportation technologies allow for transportation of resources between spatial zones. Two types of transportation technology are modelled:

- Transportation technologies without storage (e.g. electricity transmission);
- Transportation technologies that include in-built storage (i.e. linepack in gas transmission pipelines).

Transportation technologies without linepack

Transport technologies that do not include linepack are electricity transmission lines and CO_2 pipelines. These are represented with transmission lines / pipelines connecting two specific zones. Electricity transmission cost and loss data was estimated from [57] and [58]. CO_2 pipeline data was estimated from the HyNet NW project [53] and the Zero Emissions Platform [47]. Data for these technologies are shown in Table B.16.

Existing electricity transmission lines are also included, taken from Samsatli et al. [12]. The existing transmission lines are illustrated in Figure B-2.

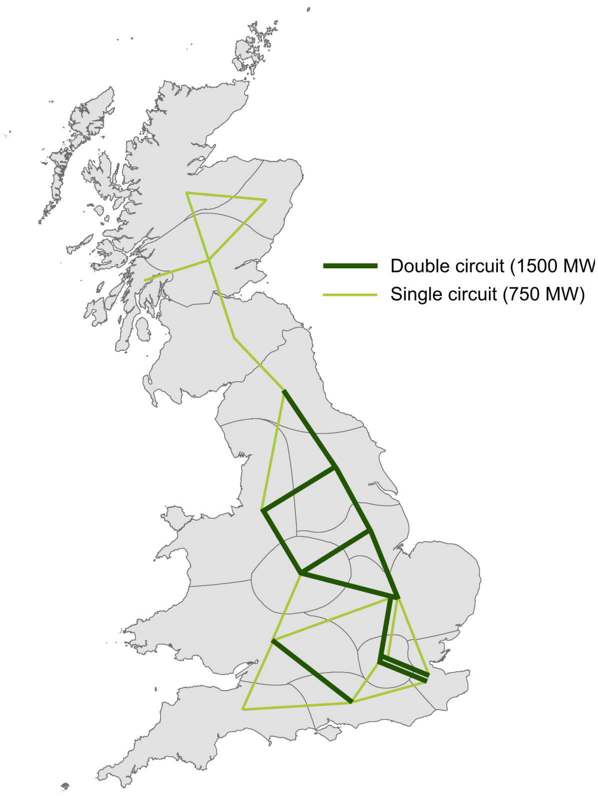


Figure B-2: Existing electricity transmission capacity between zones [12].

Table B.17: Linepack systems data. Values are per-connection: multiple connections can be installed in each zone, and the overall linepack storage capacity is the sum of all connection capacities. Data calculated from [21, 59, 60].

Technology		Natural Gas Transmission	H2 Transmission
Max injection rate (MW)		7,270	4,650
Max withdrawal rate (MW)		7,270	4,650
Max storage capacity (MWh)		11,800	2,010
Min storage capacity (MWh)		10,800	1,840
Operating flexibility		Hourly	Hourly
Capex (£M2017)		151	151
Fixed opex (£M2017/yr)		3.0	3.0
Variable opex (£2017/MWh)		Negligible	Negligible
Lifetime (yrs)		40	40
Cost	2030	1.00	1.00
learning	2040	1.00	1.00
factor	2050	1.00	1.00

Transmission systems with linepack

Transmission systems with in-built storage (linepack) are modelled differently, based around a centralised transmission system, to which pipelines can be built connecting the transmission system to a given zone. Each pipeline has a transportation and storage capacity associated with it, and multiple pipelines can be built in a zone to increase both the transportation capacity into and out of the zone, and also the overall storage capacity of the transmission system.

In reality, transmission systems consist of many pipes of various sizes and lengths, but in the VWM, all individual pipes are representative of a 762 mm (30") diameter pipe of 75 km in length. These values were chosen based on data for the existing GB natural gas National Transmission System (NTS) [59, 60]: these values, in combination with the numbers of existing connections defined in Table B.18, result in overall linepack storage and energy delivery capacity per zone of a similar size to the existing NTS. Capacities for the hydrogen system are estimated from the natural gas data based on the lower energy density of hydrogen. Cost data is from [21]. This data is presented in Table B.17.

The existing natural gas transmission system is included in the model with a representative number of connections to provide realistic overall linepack capacity and maximum flow rates between zones. The number of existing connections per zone for the natural gas transmission system is shown in Table B.18. This data was based on shapefiles of the NTS from the National Grid [59], and data on the overall linepack of the NTS [60].

Table B.18: Existing natural gas linepack (transmission system) connections in each zone. Estimated from [59, 60].

	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
Number of connections	0	16	0	23	19	13	45	32	8	11	63	23	4	13	4	5

B.2 Experimental Design, Materials, and Methods

B.2.1 Representation of space and time

The data presented in this article, in particular the resource data, is focussed on the GB energy system, and presented in the spatio-temporal resolution used in the VWM in the main article [61].

Spatially, the GB energy system is represented with 16 spatial zones, based on the zones used in the National Grid Seven Year Statement [62]. Figure B-3 shows a map of these zones.

A temporal aggregation is used in order to represent the time-varying data across the time horizon modelled. Details of the aggregation are shown in Figure B-4. Each yearly interval that is modelled is represented with five seasonal intervals, including the four main seasons and a short "peak" interval to represent energy demands on extreme occasions. Within each season, the sub-daily variation is modelled with four sub-day intervals (enabling, for example, the representation of peak energy demands in the morning and evening). Multiple yearly intervals are also modelled, and can include changes in the overall level of resource availability/demand, and changes in technology parameters (e.g. costs).

The resource data in this article has been aggregated to fit the spatio-temporal representation used. For spatial data, either zonal average or centroidal data has been used. For temporal data, typically data has been averaged across each time interval; where alternative methods have been used, this is described in the following sections.

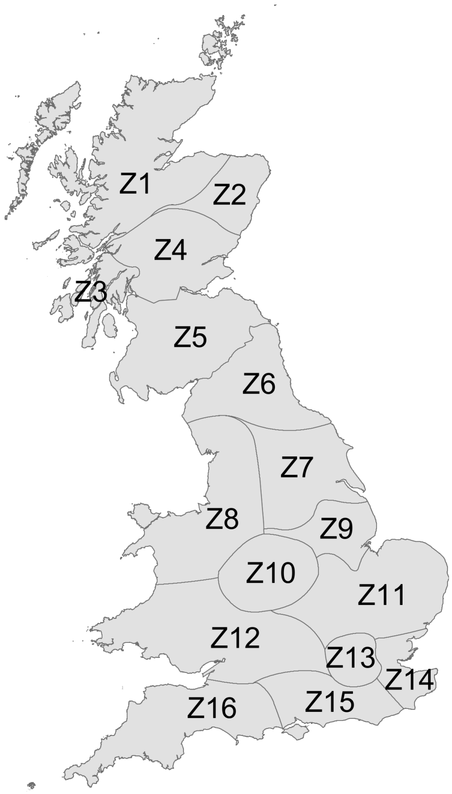


Figure B-3: Spatial zones used to represent the Great Britain energy system. Based on the National Grid Seven Year Statement zones [62]

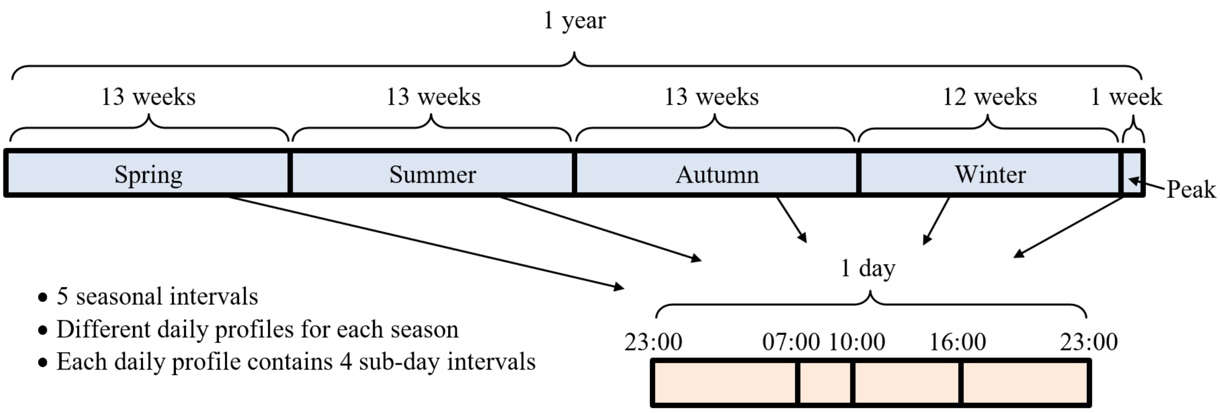


Figure B-4: Details of the temporal aggregation

B.2.2 Wind speed processing

Hourly wind speeds across an entire year were extracted from the Renewables Ninja database [4] for each spatial zone. Averaging wind speeds across a day or season would not represent the variability of the wind realistically, therefore "typical" wind speed profiles were generated for each season. For each zone, and for each seasonal interval, "typical" days were selected, by comparing the standard deviation of wind speed on each day to the average standard deviation across the season. The wind speeds on each typical day were then scaled to match the average wind speed across the season. Hence, an hourly profile is generated for each season that accurately represents the average wind speed for the season, and approximates the expected level of wind speed variability on a typical day. For the peak season, hourly data from winter was used, but scaled to equal the lower quartile daily wind speed for winter (rather than the average), therefore representing a possible low-wind day. Finally, data was aggregated to the model time representation by taking the average wind speed across all hours within each model hourly time interval. This procedure was carried out for both offshore and onshore locations. The generated representative wind speeds would result in approximate average annual load factors across all zones of 24% for onshore (maximum of 31% in zone 16), and 41% for offshore (maximum of 50% for zone 1).

B.2.3 Solar resource processing

The Renewables Ninja database for solar irradiance already takes into account several factors, including: solar irradiance, the sun's position, ambient temperature, the PV panel's location and orientation, and real solar farm data [63]. Data from the MERRA-2 database for 2014 was used, and a panel tilt of 40° was assumed. Hourly data from the centroid of each spatial zone across one year was extracted.

To aggregate the data to the model temporal resolution, hourly data was averaged for each season (the peak season was assumed to have the same hourly profile as the winter season), and averaged across all hours within each sub-day interval.

The data results in an average capacity factor for the country (not accounting for ancillary losses) of 13.3%. The highest capacity factor is achieved in Zone 14 (South East England), with a capacity factor of 16.0%.

B.2.4 Wind and solar existing installed capacities

Data for the existing installed capacity of wind turbines was collated from the BEIS Renewable Energy Planning Database [31]. The installed capacity of both offshore and onshore wind turbines for each spatial zone was collated based on the location information provided in the database. Only wind projects that are currently operational or under construction were included. Retirement dates were estimated based on the date upon which the project was operational, assuming a 20 year lifetime. Projects still under construction were assumed to become operational in 2020. Therefore all existing wind turbines in 2020 were assumed to have retired by 2040. Projects operational before 2005 were excluded.

As with new solar PV, existing solar installations are modelled with a representative size of 1 MW. Data for the existing installed capacity of large scale solar PV (i.e. solar farms) was collated from the BEIS Renewable Energy Planning Database [31]. Only solar installations that are currently operational or under construction were included. Retirement dates were estimated based on the date upon which the project was operational, assuming a 20 year lifetime. Projects still under construction were assumed to become operational in 2020. Therefore all existing solar installations in 2020 were assumed to have retired by 2040. Projects operational before 2005 were excluded. The total installed capacity of rooftop solar was based on the installed capacity of solar PV receiving the feed-in tariff in the BEIS Solar photovoltaics deployment database [32]. The spatial distribution of installed rooftop solar was approximated based on a combination of the land area covered by buildings in each zone and the distribution of solar farms. Retirements of existing rooftop solar were all assumed to occur in 2040.

B.2.5 Conversion technologies installed capacities

The existing installed capacity of natural gas CCGTs was obtained from BEIS data [15]: all CCGTs commissioned since 2005 were included. For inclusion in the VWM, a representative number of the CCGT technology described in Table B.11 were included to give a similar power capacity per zone. No OCGTs have been commissioned since 2005, hence no existing OCGTs data was included.

Approximate data for existing natural gas heating technologies is also included, although there is limited data available for this. Only natural gas technologies are included, as these are a) predominant, and b) the most significant to the decarbonisation challenge. For (high temperature) industrial heating, it is assumed that approximately 50% of demand is currently satisfied by

Table B.19: Number of households in each spatial zone [35, 64].

Number of households (thousands)	Z1	Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16
2020	56	232	21	658	1,320	1,376	2,460	3,591	598	2,909	2,237	2,732	4,404	1,094	1,896	1,420
2030	60	249	23	704	1,413	1,473	2,633	3,843	640	3,114	2,394	2,923	4,713	1,171	2,029	1,520
2040	64	265	24	750	1,506	1,569	2,805	4,094	681	3,317	2,550	3,114	5,021	1,247	2,162	1,619
2050	68	282	26	797	1,599	1,667	2,979	4,350	724	3,524	2,709	3,309	5,334	1,325	2,297	1,720

natural gas, based on data from [33] and the BEIS Heat Strategic Options Project [20]. Therefore, existing natural gas heating technologies are included in sufficient numbers to satisfy this demand, with half assumed to retire within one decade, and the remainder within two decades.

For domestic and commercial heating, it is assumed that the proportion of heating that is satisfied by natural gas is equal to the proportion of buildings connected to the gas grid, as provided by [34]. Hence, the number of existing technologies for domestic heating is calculated from the proportion of buildings on the gas grid and the number of households in each zone.

The number of households in each spatial zone was calculated from data from the Office for National Statistics (ONS) for 2016 [35]. For each decade, the number of households is scaled based on ONS projections for the overall number of households (England only) [64]. This supporting data is shown in Table B.19.

Finally, the number of existing commercial heating technologies is calculated from the peak demand, the maximum operating rate of the gas-based technologies, and the proportion of buildings on the gas grid. Half of existing gas boilers are assumed to retire in 2030, the other half in 2040.

B.3 Additional data used in Chapter 6

The dataset described above was used for the study presented in Chapter 5 of this thesis. The same dataset was used for Chapter 6, with some minor alterations; notably including some bioenergy value chains. The data assumptions for these additions are provided in this section.

B.3.1 Bioenergy value chains

Two bioenergy value chains were modelled in Chapter 6: conversion of biogenic waste to biomethane and gasification of a biomass crop to produce hydrogen.

A representative conversion technology was modelled for conversion of biogenic waste to biomethane, representing a biogas plant that carries out anaerobic digestion of waste to biogas and upgrading of biogas to biomethane. The produced biomethane is indistinguishable from natural gas (which is predominantly methane) in the model. Key data for the anaerobic digestion & biogas upgrading plant are taken from [65] and are shown in Table B.20.

A total availability of biogenic waste of 36.5 Mt/yr was assumed, allowing for biomethane production of up to 21 TWh/yr, as in [43]. This waste availability is shared amongst all 16 spatial zones, with the availability assumed to be proportional to total electricity demand in the zone (i.e. electricity demand and waste generation are both dependent on the population in the same way). Utilisation of the waste receives a gate-fee revenue of £25/t. The entire waste-to-biomethane value chain, including end use of the biomethane, was modelled with a CO_2 impact of zero, in accordance with UK government guidance for CO_2 accounting of biogas [66].

The other bioenergy value chain modelled in this study represents conversion of "non-waste" biomass to hydrogen. A generic biomass energy crop was modelled, using data representative of a miscanthus-type crop. The crop can be converted to hydrogen through a gasification plant that includes CO_2 capture at a rate of 91%.

The biomass crop is assumed to have a yield of 35 MWh/ha/yr, which includes energy requirements for processing into pellets. The cost of biomass pellets was assumed to be £24/MWh [67, 68], which includes all costs upstream of the gasification plant, i.e. biomass cultivation, processing and transportation. Available land for growing crops was taken from [2], where it was assumed that the crop would be grown on grassland and a GIS analysis of GB was used to find available land.

For the first decade (2020-2030), it was assumed that only 18% of the total suitable land could be used for bioenergy, giving rise to a primary energy availability of 20 TWh/yr. This constraint is relaxed in each decade, reaching a limit of 58% of suitable land in the final decade (2050-2060), giving rise to a primary energy availability of 64 TWh/yr. This availability is in line with Committee on Climate Change estimates [43, 68].

The biomass gasification to hydrogen is based on data for the integrated gasification combined cycle (IGCC) with CO_2 capture (excluding the power island) in [67]. Key data for this technology are shown in Table B.20.

Assessing the value chain impacts of bioenergy crops is complex, as biomass cultivation can have far-reaching impacts, including on greenhouse gas emissions, water usage, food security and soil erosion [69]. Furthermore, the magnitudes of these impacts will vary depending on which of the various crops and land types are used.

Estimates for the CO_2 impacts of bioenergy crops vary widely. Typically, it is assumed that the CO_2 released when biomass is converted to another energy form (e.g. through combustion or gasification) is balanced by the CO_2 consumed by the crop during growth. Hence, if CO_2 capture is used at the energy conversion stage, it may be possible to achieve net negative emissions. This is the reason for the strong interest in Bioenergy with CCS (BECCS) for future energy systems [70].

However, bioenergy value chains have other CO_2 impacts, arising from the crop cultivation, processing and transportation for example. Depending on the crop used and processing and transport required, estimates for the CO_2 impacts of these stages range between 20 and 240 $kgCO_2$ per MWh of biomass [70]. Moreover, further CO_2 impacts may arise from converting land to grow energy crops (land use change emissions). These emissions depend heavily on the land type, with estimates of 0-0.07 tCO_2/ha for marginal land, 75-200 tCO_2/ha for grassland, 350-720 tCO_2/ha for forest, and in excess of 1,000 tCO_2/ha for wetland [70]. Further emissions may also arise from land-use change elsewhere as a consequence of the primary land use changes, known as "indirect" land use change emissions.

Clearly, bioenergy value chains are complex and it is important that they are designed carefully to ensure that their overall system impact is positive. However, optimisation of bioenergy value chains was not the focus of this study. Instead, the reason for including bioenergy in this study is to explore the implications of bioenergy value chains with the potential for net-negative emissions on the role of hydrogen in the energy system.

In Chapter 6, the CO_2 impact of producing the biomass pellets, including cultivation, processing and transportation, but excluding CO_2 consumed by the crop during growth, was assumed to be 130 $kgCO_2$ per MWh of biomass. Assuming that the CO_2 consumed by the crop during growth is equal to the CO_2 emitted during gasification (before CO_2 capture), and with the conversion technology details in Table B.20, this results in a net CO_2 impact for the hydrogen produced from biomass of –610 $kgCO_2$ per MWh of hydrogen.

Table B.20: Model input data for bioenergy conversion technologies.

	Anaerobic digester + upgrade to biomethane	Gasification to hydrogen
Input resource	Biogenic waste	Biomass pellet
Output resource	Methane	Hydrogen
Conversion efficiency	0.57 MWh_{CH4}/t_{waste}	0.34 MWh_{H2}/MWh_{pellet}
CO_2 capture rate	*See Note 1*	0.10 tCO_2/MWh_{H2}
CO_2 emission rate	*See Note 1*	1.00 tCO_2/MWh_{H2}
Maximum operating rate (MW output)	8.4	358.0
Minimum operating rate (MW output)	4.2	179.0
Plant capex (£M)	18.5	556
Plant fixed opex (£M/yr)	4.7	27.8
Plant lifetime (yr)	20	25
Reference	[65]	[67]

Note 1 - Anaerobic digester plant emissions are modelled as zero, as it is assumed that any CO_2 emitted along the biogas value chain is biogenic [66].

B.3.2 Hydrogen fuel cells

Hydrogen fuel cells are an interesting option for generation of electricity and heat from hydrogen, as they have the potential to achieve high efficiencies with flexible operation. Worldwide there are relatively few large-scale fuel cell installations, although there are several in South Korea, including a 59 MW plant (the world's largest) [71].

The data for hydrogen fuel cell plants in the VWM were updated in Chapter 6, based on a state-of-the-art commercially-available fuel cell system [72]. Two sizes of fuel cell plant are modelled, with maximum electricity outputs of 10 MW and 100 MW. Each plant requires 1.67 MWh of hydrogen per MWh of electricity produced and also produces 0.2 MWh of heat, that for example can be used for district heating [72]. The fuel cells have a lifetime of 10 years and can be operated flexibly. Plant costs have been estimated from [41]: the 10 MW plant has a modelled capex of £35m in 2020, falling to £21m in 2050; the 100 MW plant has a capex of £320m in 2020, falling to £192m in 2050. The plant fixed opex is assumed to be 4% of the capex.

B.3.3 Other data alterations

Two other alterations were made to the previous model dataset:

- The fixed operating costs for natural gas (and hydrogen) distribution grids were reduced from 3% of capex to 1% of capex, giving a new operating cost for each MW of grid capacity of £13,400 per year. This results in a more representative figure for the average operating costs per customer [73].

- As four decades were modelled in this study, estimates for the future cost of producing or importing natural gas were included, based on the base case in the National Grid Future Energy Scenarios [74]. The cost in the first decade (2020-2030) is £18.10/MWh, rising to £23.90/MWh by the final decade (2050-2060).

Appendix C

Calculating the effect of hydrogen injection on gas pipelines

In this appendix, the full calculations that were used to estimate the effect of hydrogen injection on pipeline energy delivery and linepack in Chapter 5 are presented. This information was originally published as supplementary material to the article that is presented Chapter 5 [61].

Pipeline energy delivery

The energy delivery rate (i.e. the power, in MW) of gas in a pipeline can be expressed as follows:

$$H = u_n Q_n \tag{C.1}$$

where H is energy delivery rate; u_n is the gas energy density at Standard Temperature and Pressure (STP); and Q_n is the volumetric flow rate at STP. Therefore, the relative energy delivery of a pipeline carrying hydrogen (or a methane-hydrogen mixture) compared to the same pipeline carrying methane can be expressed as follows:

$$\frac{H_{mix}}{H_{CH4}} = \frac{u_{n,mix}}{u_{n,CH4}} \frac{Q_{n,mix}}{Q_{n,CH4}} \tag{C.2}$$

The energy density of the mixture gas, $u_{n,mix}$, can be calculated using a simple mixing rule, from the energy densities of methane and hydrogen ($u_{n,CH4}$ and $u_{n,H2}$, respectively) and the volume fraction of hydrogen in the mixture (ϕ):

$$u_{n,mix} = \phi u_{n,H2} + (1-\phi)u_{n,CH4} \tag{C.3}$$

The values used for u_{H2} and u_{CH4} are shown in Table C.1.

Table C.1: Key gas properties for methane and hydrogen, used to calculate energy flow rate [75, 76, 77]

Property	Symbol	Unit	Methane (CH_4)	Hydrogen (H_2)
Energy density (STP)	u_n	J/m^3	3.58 $\times 10^7$	1.08 $\times 10^7$
Specific gravity	S	-	0.5537	0.0696
Compressibility factor (7 bar)	Z_{7bar}	-	0.980	1.004
Compressibility factor (30 bar)	Z_{30bar}	-	0.920	1.018
Compressibility factor (80 bar)	Z_{80bar}	-	0.789	1.049
Kinematic viscosity (STP)	ν	m^2/s	1.52 $\times 10^{-5}$	9.85 $\times 10^{-5}$

The volumetric flow rate can be calculated using the general flow equation for steady state gas flow (here assuming a horizontal pipe) [78]:

$$Q_n = \left(\frac{\pi^2 \rho_{air}}{64}\right)^{\frac{1}{2}} \frac{T_n}{p_n} \left(\frac{(p_1^2 - p_2^2)D^5}{fSLTZ}\right)^{\frac{1}{2}} \tag{C.4}$$

where ρ_{air} is the density of air at STP; T_n and p_n are the gas temperature and pressure at STP; p_1 and p_2 are the inlet and outlet pressures; D is the pipe diameter; f is the friction factor; S is the gas specific gravity; L is the pipe length; T is the gas temperature; and Z is the gas compressibility factor.

By dividing equation (C.4) for the mixture gas by the same equation for methane, and assuming that the same pipeline, with the same pressure drop, is considered in both cases, and that the temperature is unchanged between the gases, a simplified expression for the relative volume flow rate of the mixture gas compared to methane is obtained:

$$\frac{Q_{n,mix}}{Q_{n,CH4}} = \left(\frac{f_{CH4} S_{CH4} Z_{CH4}}{f_{mix} S_{mix} Z_{mix}}\right)^{\frac{1}{2}} \tag{C.5}$$

Values for S_{mix} and Z_{mix} can be reasonably estimated using a mixing rule, in the same manner as equation (C.3) [79]; the values used for hydrogen and methane are provided in Table C.1.

The friction factor however depends on the gas flow regime and therefore cannot be linearly approximated in the same manner. For normal operation of gas transmission and distribution pipelines, Reynolds numbers (Re) are typically below 10^6, and relative roughnesses are low, so "smooth pipe" flow is assumed (i.e. pipe wall friction is small compared to fluid friction). In this case, the friction factor can be expressed as follows [80]:

$$f = 0.079 Re^{-\frac{1}{4}} \tag{C.6}$$

The Reynolds number is given by:

$$Re = \frac{4Q_n}{\pi D \nu} \tag{C.7}$$

where ν is the gas kinematic viscosity.

Combining equations (C.6) and (C.7), the friction factor can be expressed as follows:

$$f = 0.056 \left(\frac{\pi D \nu}{Q_n} \right)^{\frac{1}{4}} \tag{C.8}$$

Therefore the relative friction factor of the pipeline carrying mixture gas compared to the pipeline carrying methane is given by:

$$\frac{f_{mix}}{f_{CH4}} = \left(\frac{\nu_{mix}}{\nu_{CH4}} \frac{Q_{n,CH4}}{Q_{n,mix}} \right)^{\frac{1}{4}} \tag{C.9}$$

Thus, using equation (C.9), the friction factor can be eliminated from equation (C.5). The resulting expression for the relative volume flow rate is as follows:

$$\frac{Q_{n,mix}}{Q_{n,CH4}} = \left(\frac{S_{CH4}}{S_{mix}} \frac{Z_{CH4}}{Z_{mix}} \right)^{\frac{4}{7}} \left(\frac{\nu_{CH4}}{\nu_{mix}} \right)^{\frac{1}{7}} \tag{C.10}$$

Finally, the relative energy delivery can then be expressed as follows:

$$\frac{H_{mix}}{H_{CH4}} = \frac{u_{n,mix}}{u_{n,CH4}} \left(\frac{S_{CH4}}{S_{mix}} \frac{Z_{CH4}}{Z_{mix}} \right)^{\frac{4}{7}} \left(\frac{\nu_{CH4}}{\nu_{mix}} \right)^{\frac{1}{7}} \tag{C.11}$$

The value of ν_{mix} can be estimated using the mixing rule shown in equation (C.3), and values for ν_{CH4} and ν_{H2} are shown in Table C.1.

Linepack

The relative usable linepack flexibility of a pipeline with a hydrogen-methane mixture compared to the same pipeline with pure methane was estimated based on the equations presented by Haeseldonckx and d'Haeseleer [81].

The usable linepack flexibility of a pipeline in energy terms can be calculated from the volumetric linepack flexibility at STP ($V_{flex,n}$) and the gas energy density (u_n):

$$E_{flex} = u_n V_{flex,n} \tag{C.12}$$

The volumetric linepack flexibility V_{flex} can be expressed as follows [81]:

$$V_{flex,n} = V_{geom} \left(\frac{p_m}{Z_m} - \frac{p'_m}{Z'_m} \right) \frac{1}{p_n} \frac{T_n}{T} \tag{C.13}$$

where V_{geom} is the geometric pipe volume; p_m and p'_m are the upper and lower mean pipeline pressures respectively; and Z_m and Z'_m are the corresponding gas compressibilities at the upper and lower mean pressures. The upper and lower mean pressures refer to the two pressure states between which the pipeline linepack is swung for flexibility. These mean pressures are calculated from the pipeline inlet and outlet pressures (p_1 and p_2):

$$p_m = \frac{2}{3} \left(p_1 + p_2 - \frac{p_1 p_2}{p_1 + p_2} \right) \tag{C.14}$$

Combining equations (C.12) and (C.13):

$$E_{flex} = u_n V_{geom} \left(\frac{p_m}{Z_m} - \frac{p'_m}{Z'_m} \right) \frac{1}{p_n} \frac{T_n}{T} \tag{C.15}$$

Finally, to compare the available linepack flexibility of a pipeline with different gases, but under the same pressure conditions, equation (C.15) for the mixture gas can be divided by the same equation for methane, with several terms being eliminated:

$$\frac{E_{flex,mix}}{E_{flex,CH4}} = \frac{u_{n,mix}}{u_{n,CH4}} \frac{\left(\frac{p_m}{Z_{m,mix}} - \frac{p'_m}{Z'_{m,mix}}\right)}{\left(\frac{p_m}{Z_{m,CH4}} - \frac{p'_m}{Z'_{m,CH4}}\right)} \tag{C.16}$$

Appendix D

Sensitivities studies for Chapter 6

In addition to the 15 scenarios that were described in detail and modelled in Chapter 6, a further 23 scenarios were modelled to explore sensitivities for two critical input data: the discount rate, and the heat pump coefficient of performance. Details of these sensitivities are provided in this appendix.

D.1 Discount rate

D.1.1 Sensitivity scenarios

In the main scenarios that were modelled in this study, a discount rate of 3.5% was used, following UK government guidance [82]. However, as discussed in the main text, the choice of discount rate can significantly influence results when considering decarbonisation decisions over long time periods. Therefore additional sensitivity scenarios with different discount rates were modelled in order to assess the impact of the discount rate on the scenario results. Scenarios with discount rates of 0.1% and 8% were modelled. All of the scenarios with policies focussing on decarbonisation, detailed in Table 3 of the main text, were repeated with these alternative discount rates. Consequently, 14 additional scenarios were modelled.

D.1.2 Results

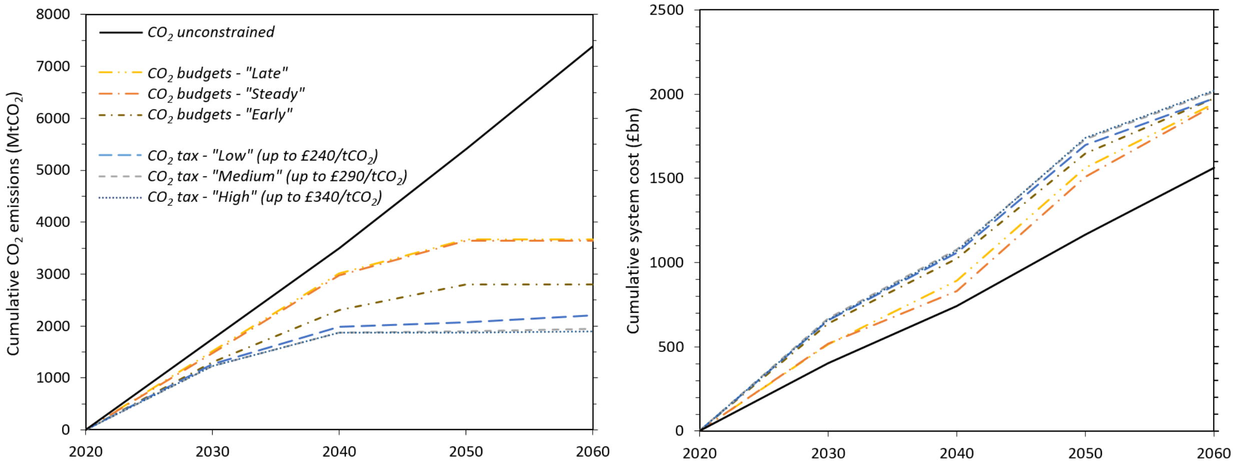
The results for the sensitivity runs with a discount rate of 0.1% are shown in Figure D-1; equivalent results for a discount rate of 8% are shown in Figure D-2. Finally, Figure D-3 provides overall (discounted) cost and CO_2 results, and the average cost of CO_2 savings, for each scenario.

The discount rate determines the importance of future costs relative to present day costs. With a discount rate of 0.1%, future costs have almost equal weighting to present-day costs in the optimisation objective function, whilst with higher discount rates the importance of future costs falls.

In the case of CO_2 budgets, this effect means that with higher discount rates, investment in decarbonisation is delayed until it is essential, as the associated costs are seen to reduce. The level of "voluntary" early decarbonisation, i.e. the reduction in CO_2 emissions in a given decade beyond what is required by the CO_2 budget, is notably higher in the cases with lower discount rates. With a discount rate of 0.1% for example, as Figure D-1 shows, CO_2 emissions in the "late" CO_2 budgets scenario follow a very close trajectory to the "steady" scenario, despite having not being required to by the CO_2 budgets. Examples of this voluntary early decarbonisation include earlier investment in renewable electricity generation and long-life infrastructure such as electricity distribution networks. As can be seen in Figure D-3(b), the result of this earlier decarbonisation is a lower overall level of CO_2 emissions. For example, in the "late" CO_2 budgets cases, overall emissions are 21% lower with a discount rate of 0.1% than with a discount rate of 3.5%, and 27% lower than with a discount rate of 8%.

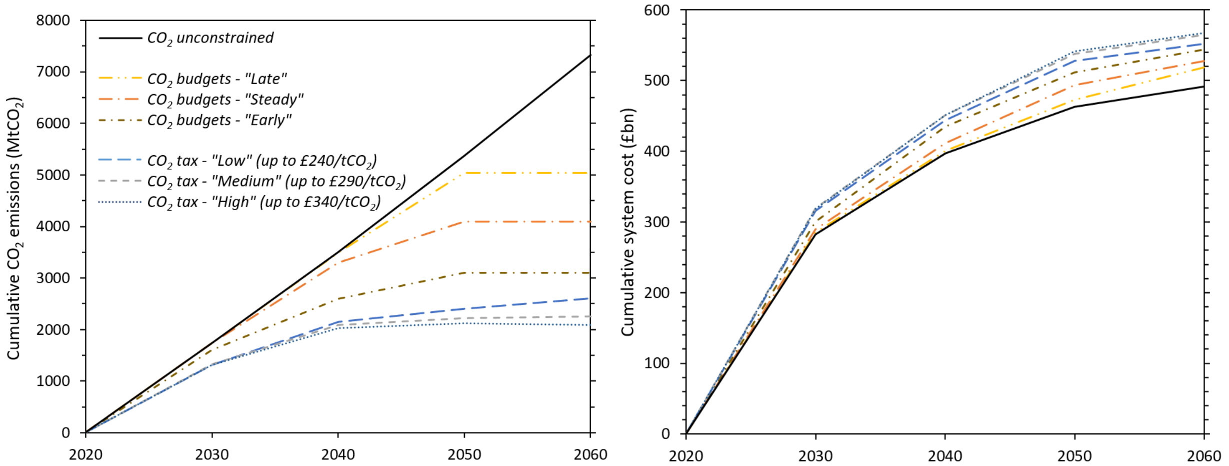
The discount rate has a less significant effect on the scenarios with CO_2 taxes, however a lower discount rate does appear to increase the potency of a tax. For example, with a discount rate of 0.1%, a CO_2 tax of £290/tCO_2 is sufficient to achieve net-zero emissions by 2050-2060, whilst in the scenarios with higher discount rates, a tax rate of £340/tCO_2 is necessary.

Finally, given that the majority of spending on decarbonisation occurs in later decades, the effect of the discount rate in all scenarios is to reduce the apparent costs of this decarbonisation. Figure D-3(c) shows the average costs of CO_2 reductions for each scenario (as defined in Equation 6 of the main text). For each discount rate, this cost is calculated with respect to the "CO_2 unconstrained" scenario with the same discount rate. As Figure D-3(c) shows, the average CO_2 costs range widely, from a maximum of £12/tCO_2 in the cases with a discount rate of 8% to a maximum of £103/tCO_2 in the cases with a discount rate of 0.1%.



(a) (b)

Figure D-1: Cumulative CO_2 emissions (a) and costs (b) in scenarios with decarbonisation policies and a discount rate of 0.1%. Costs are overall system costs, discounted to 2020.



(a) (b)

Figure D-2: Cumulative CO_2 emissions (a) and costs (b) in scenarios with decarbonisation policies and a discount rate of 8%. Costs are overall system costs, discounted to 2020.

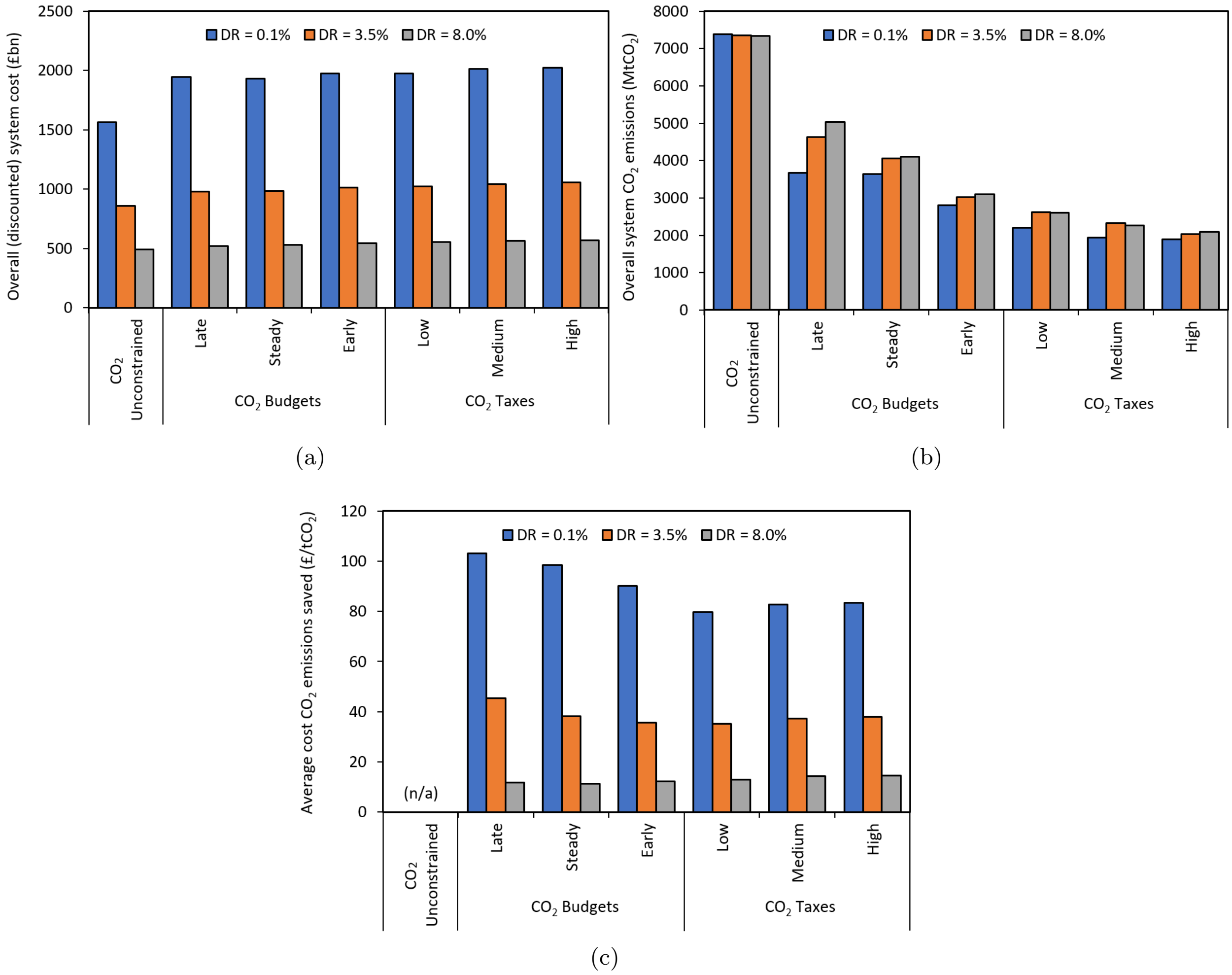


Figure D-3: Cost and CO_2 results for scenarios with decarbonisation policies and of discount rates of 0.1%, 3.5% and 8%: (a) Overall (discounted) system cost; (b) Overall system CO_2 emissions; (c) Average cost of CO_2savings

D.1.3 Conclusion

These results show the importance of the discount rate when considering investment decisions over long time periods. Whilst it is difficult to know what the most appropriate discount rate is for a given assessment, it is essential that the discount rate is taken into consideration when interpreting scenario results.

D.2 Electric heat pump coefficient of performance

D.2.1 Sensitivity scenarios

In the scenario results presented in the main article, electric heat pumps were found to have a high contribution to the decarbonised energy system. In the "steady" CO_2 budgets case, for example, 87% of domestic and commercial heat demands in 2050-2060 were satisfied by electric heat pumps. In the context of heat provision, electric heat pumps are an alternative to hydrogen, and therefore the uptake of hydrogen is likely to be adversely affected by their uptake. Therefore, the modelling assumptions behind electric heat pumps should be considered carefully.

The coefficient of performance (COP) represents the amount of heat energy delivered per unit of electrical energy input. Since heat pumps can have COPs in excess of two, this means they have an apparent efficiency of greater than 100% (whereas alternative technologies all have efficiencies lower than 100%) and thus the value of the COP is a key assumption for modelling heat pumps. In the main scenarios that were modelled in this study, the COP was assumed to be 2.5 for domestic electric heat pumps and 4 for commercial electricity heat pumps, based on values in the literature [43, 33]. As a sensitivity study, further scenarios were modelled in which the COP was set to 2 for both domestic and commercial heat pumps. The "steady" CO_2 budgets case and all of the scenarios with specific policies for incentivising hydrogen were included in this sensitivity study, in order to explore the effect of the COP assumption on hydrogen uptake.

D.2.2 Effect on heat pump and hydrogen uptake

The results from these sensitivity scenarios are shown below. Figure D-4 shows the overall provision of domestic and commercial heat in 2050-2060 in each of the scenarios, for both the original scenarios and the sensitivity scenarios with reduced heat pump COPs. Figure D-5 shows results for hydrogen uptake in the sensitivity scenarios (the equivalent results for the original scenarios are shown in Figure 6 of the main text). Figures D-4 and D-5 suggest that the heat pump COP does have an impact on hydrogen uptake, but that it is relatively small.

The impact of the reduced heat pump COP is most significant in the domestic sector and in the cases with less hydrogen uptake overall. In the "steady" CO_2 budgets cases, for example, use of hydrogen for domestic heat is 28 TWh/yr in 2050-2060 in the case with a reduced electric heat pump COP, compared to 0.3 TWh/yr in the original scenario. Interestingly, although capital grants for hydrogen boilers were found to be relatively ineffective for incentivising hydrogen in the original runs, with a lower COP assumption their effectiveness increases. This can be seen by comparing provision of heat by hydrogen between the case with 100% capital grants and the equivalent case without this policy in place (the "steady" CO_2 budgets case): with the original heat pump COP assumptions, 100% capital grants increase hydrogen usage in domestic heat by 17 TWh/yr in 2050-2060; with reduced COP assumptions, the increase is 56 TWh/yr.

Meanwhile, as Figure D-4(a) shows, the effect of heat pump COP on hydrogen uptake is smaller in the cases that already have higher hydrogen uptake. This suggests that in these scenarios the hydrogen incentives have been effective and have already helped to overcome the cost difference between electric heat pumps and hydrogen; therefore, the reduced COP has little impact. In the cases with less support for hydrogen, the cost difference between heat pumps and hydrogen still exists in the original runs, but reducing the heat pump COP increases the competitiveness of hydrogen.

Finally, as shown in Figure D-4(b), heat pump COP also has less influence on hydrogen uptake in the commercial sector. This is partly because in the commercial sector, natural gas is also a competitive low-carbon heat source, due to the availability of natural gas combined heat and power (CHP) plants with CO_2 capture. Therefore, the reduced competitiveness of electric heat pumps tends to lead to increased natural gas usage, rather than hydrogen. In fact, in cases with obligations for hydrogen injection, hydrogen usage in the commercial sector reduces with a lower heat pump COP. This is because total hydrogen injection into the gas grid remains constant (at the level specified by the obligation) and domestic hydrogen usage becomes more favourable when the COPs are reduced; therefore, domestic usage increases and commercial usage reduces.

These results show that, to some extent, the competitiveness of heat pumps is affected by their COP. Furthermore, lower COPs for heat pumps do lead to an increase in competitiveness for hydrogen. However, in the sensitivity study performed here, the impact is relatively small. In particular, in all scenarios the overall mix of heating provision and the preferred heating technology remains unchanged when the heat pump COP is reduced.

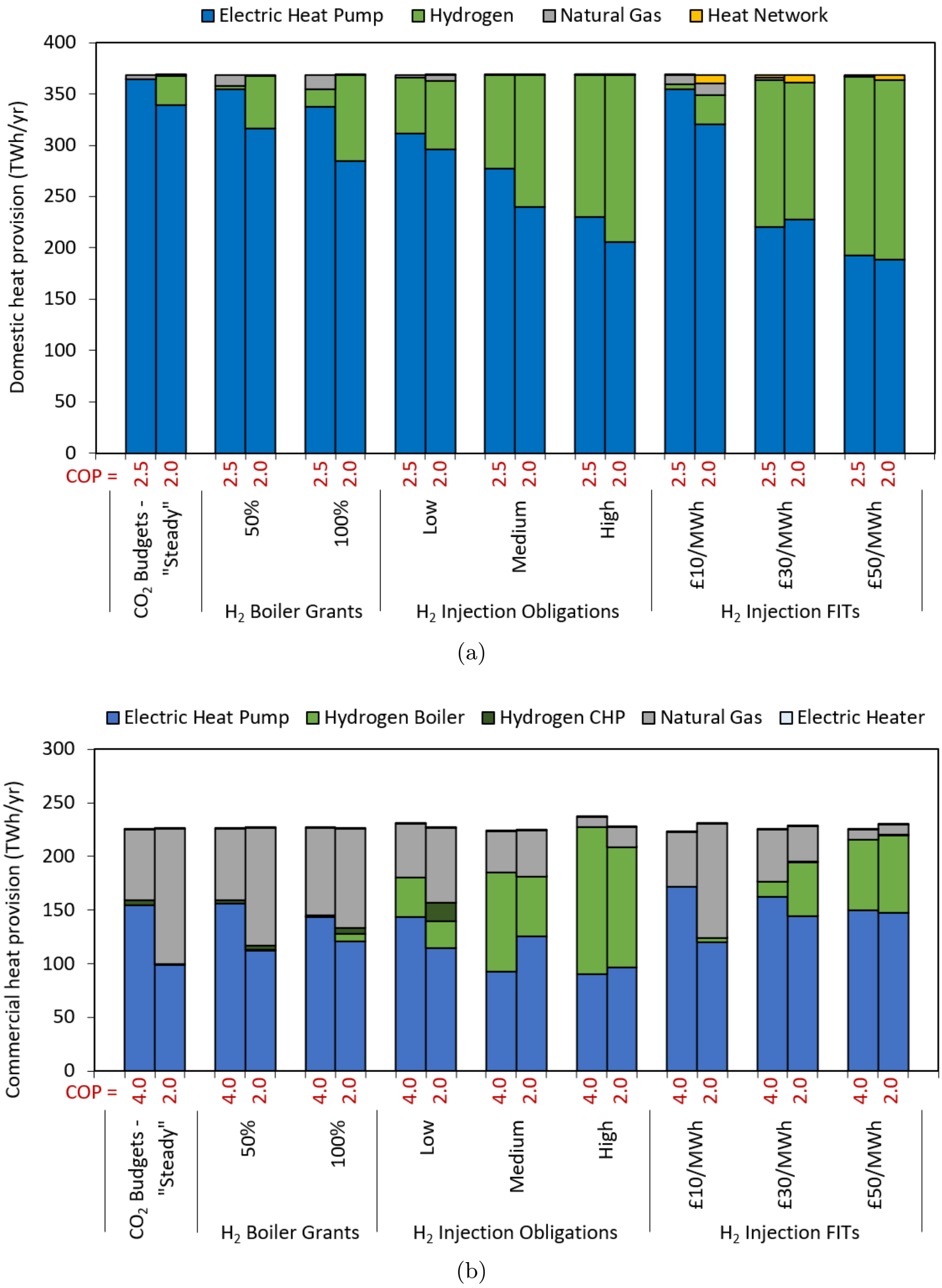


Figure D-4: Heating provision in (a) the domestic sector and (b) the commercial sector in 2050-2060 for a range of scenarios, comparing the original COPs with the sensitivity scenarios with COP = 2.

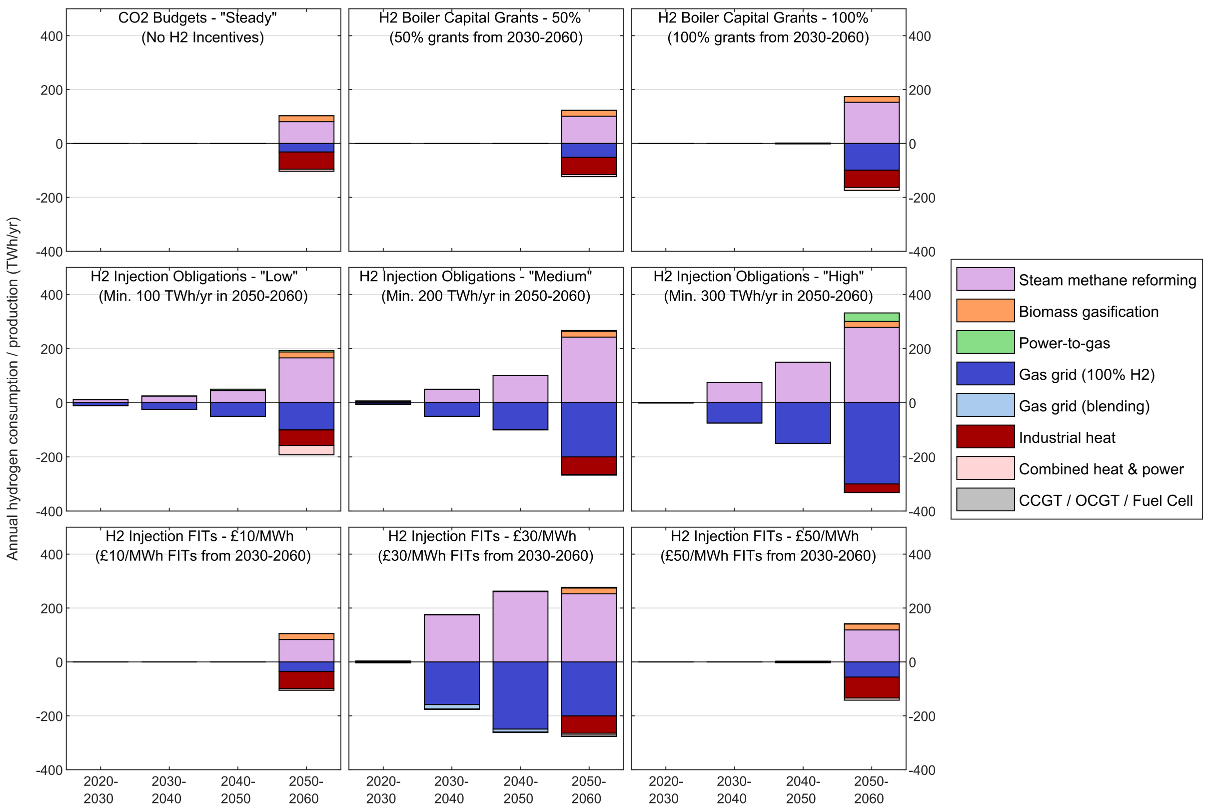


Figure D-5: Hydrogen production and consumption by technology or application in each decade, for a range of scenarios (with a heat pump coefficient of performance of 2). Positive values denote hydrogen production, negative denote consumption.

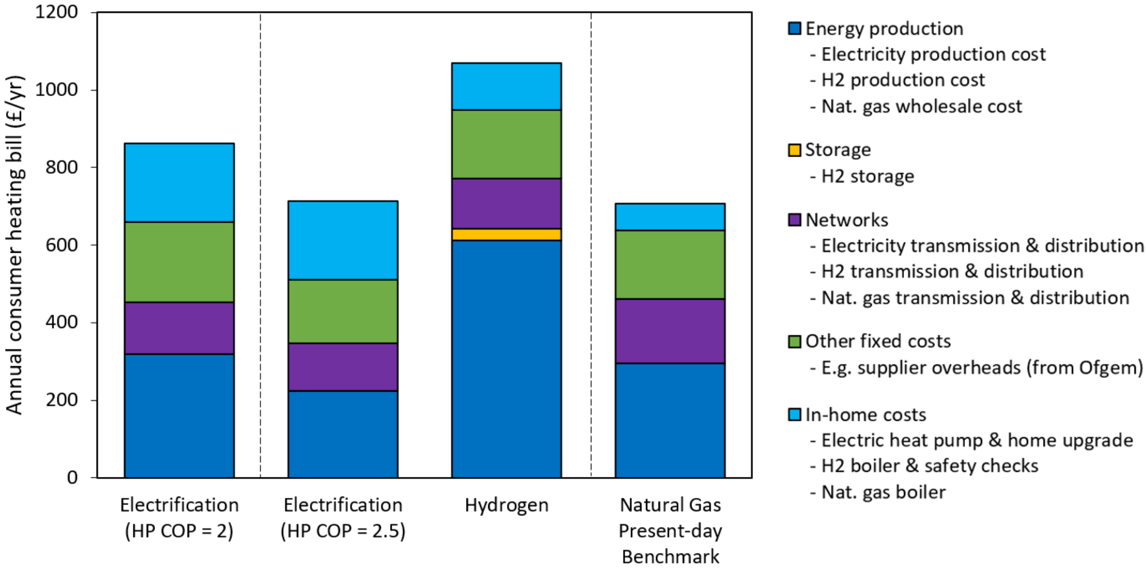


Figure D-6: Annual consumer heating costs for a range of different heating scenarios. "Electrification (HP COP = 2)" was calculated from the "steady" CO_2 budgets scenario in the sensitivity study; the remaining cases are replicated from Figure 9 in the main text.

D.2.3 Effect on consumer heating bill

Finally, a typical annual domestic heat bill was calculated from the "steady" CO_2 budgets case, with a heat pump COP of 2. This can be compared to the annual heating bills presented in Section 4.3 of the main text, including the annual heating bill for a heat pump with a COP of 2.5. The new heating bill for a domestic electric heat pump with a COP of 2 is shown in Figure D-6, with the original heating bills that were presented in the main text.

The new annual electric heat pump heating bill, with a reduced COP of 2, is 21% higher than the original electric heat pump bill, at £863/yr. This is due primarily to increased electricity demand, which is reflected in increased costs from electricity production and from the fixed costs arising from the supply of electricity (although these are "fixed" costs, it is assumed they would be shared amongst electricity users based on their electricity consumption; therefore, domestic users would pay an increased proportion of these costs if their electricity demand increased).

The new annual heating bill is now closer to, but still lower than, the annual bill that was calculated for hydrogen, which was calculated to be £1070/yr. This helps to explain the previously-discussed result, that the "smaller" hydrogen incentives become more effective when the electric heat pump COP is reduced. In the original scenarios, the difference between the electrification heating bill and the hydrogen heating bill was £355/yr; this is reduced to £207/yr with the electrification bill based on a heat pump COP of 2. This difference is easier to overcome for hydrogen incentives.

D.2.4 Conclusion

In conclusion, the reduced heat pump coefficient of performance modelled in this sensitivity study increases the consumer costs of heating using a heat pump by around 19% and, as a result, hydrogen becomes more competitive as a decarbonised heating option. This leads to greater uptake of hydrogen, in particular in cases with small but previously ineffective hydrogen incentives. However, despite the reduction in heat pump cost-effectiveness, they remain the lowest cost decarbonised heating option in the majority of cases. Therefore, the reduced heat pump COP does not lead to a significant change in hydrogen uptake in the scenario results.

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